



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 09:33 PM UTC

PDB ID : 6ZQN / pdb_00006zqn
EMDB ID : EMD-11369
Title : bovine ATP synthase monomer state 3 (combined)
Authors : Spikes, T.E.; Montgomery, M.G.; Walker, J.E.
Deposited on : 2020-07-10
Resolution : 4.00 Å(reported)
Based on initial models : 2CLY, 2V7Q

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

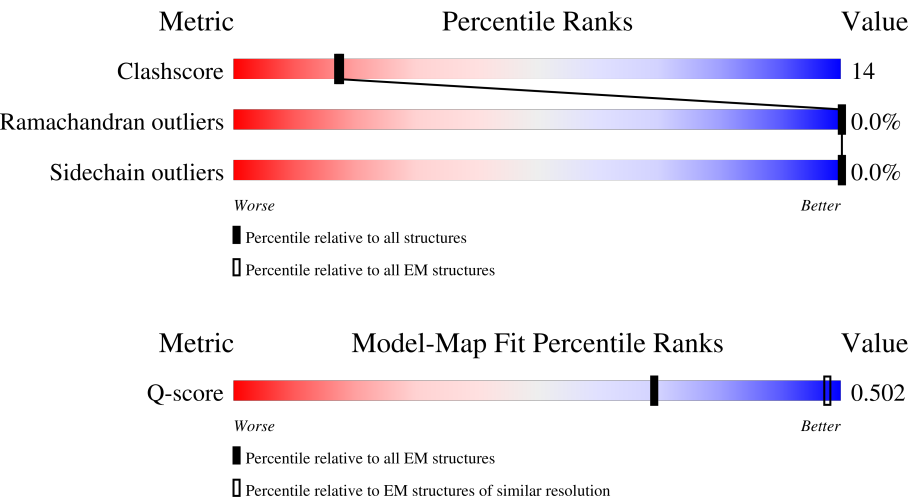
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	
1	B	510	
1	C	510	
2	D	482	

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Mol	Chain	Length	Quality of chain
2	E	482	
2	F	482	
3	G	273	
4	H	146	
5	I	50	
6	J	66	
7	K	75	
7	L	75	
7	M	75	
7	N	75	
7	O	75	
7	P	75	
7	Q	75	
7	R	75	
8	S	190	
9	8	66	
10	a	226	
11	d	160	
12	f	87	
13	g	102	
14	j	60	
15	b	214	
16	h	76	
17	k	57	
18	e	70	

2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 81277 atoms, of which 41197 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	501	Total	C	H	N	O	S	0	0
			7741	2405	3923	673	728	12		
1	B	502	Total	C	H	N	O	S	0	0
			7760	2408	3935	674	731	12		
1	C	483	Total	C	H	N	O	S	0	0
			7488	2329	3798	652	697	12		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	GLN	variant	UNP P19483
A	481	GLY	SER	microheterogeneity	UNP P19483
B	1	GLU	GLN	variant	UNP P19483
B	481	GLY	SER	microheterogeneity	UNP P19483
C	1	GLU	GLN	variant	UNP P19483
C	481	GLY	SER	microheterogeneity	UNP P19483

- Molecule 2 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	469	Total	C	H	N	O	S	0	0
			7163	2254	3605	605	688	11		
2	E	467	Total	C	H	N	O	S	0	0
			7132	2243	3593	601	684	11		
2	F	467	Total	C	H	N	O	S	0	0
			7131	2243	3592	601	684	11		

- Molecule 3 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	272	Total	C	H	N	O	S	0	0
			4300	1330	2185	368	409	8		

- Molecule 4 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	H	131	Total	C	H	N	O	S	0	0
			1940	609	970	163	196	2		

- Molecule 5 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I	47	Total	C	H	N	O	S	0	0
			764	237	395	66	64	2		

- Molecule 6 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	J	47	Total	C	H	N	O		0	0
			731	224	361	76	70			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	61	HIS	-	expression tag	UNP P01096
J	62	HIS	-	expression tag	UNP P01096
J	63	HIS	-	expression tag	UNP P01096
J	64	HIS	-	expression tag	UNP P01096
J	65	HIS	-	expression tag	UNP P01096
J	66	HIS	-	expression tag	UNP P01096

- Molecule 7 is a protein called ATP synthase F(0) complex subunit C2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	K	74	Total	C	H	N	O	S	0	0
			1079	351	550	82	93	3		
7	L	74	Total	C	H	N	O	S	0	0
			1079	351	550	82	93	3		
7	M	75	Total	C	H	N	O	S	0	0
			1095	356	558	83	94	4		
7	N	75	Total	C	H	N	O	S	0	0
			1096	356	559	83	94	4		
7	P	74	Total	C	H	N	O	S	0	0
			1079	351	550	82	93	3		
7	R	75	Total	C	H	N	O	S	0	0
			1096	356	559	83	94	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
7	O	75	Total	C	H	N	O	S	0	0
			1096	356	559	83	94	4		
7	Q	75	Total	C	H	N	O	S	0	0
			1096	356	559	83	94	4		

- Molecule 8 is a protein called ATP synthase subunit O, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	S	187	Total	C	H	N	O	S	0	0
			2989	915	1551	248	266	9		

- Molecule 9 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	8	41	Total	C	H	N	O	S	0	0
			696	231	352	52	58	3		

- Molecule 10 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	a	226	Total	C	H	N	O	S	0	0
			3611	1155	1870	276	298	12		

- Molecule 11 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	d	155	Total	C	H	N	O	S	0	0
			2549	821	1276	207	242	3		

- Molecule 12 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	f	83	Total	C	H	N	O	S	0	0
			1411	456	718	120	114	3		

- Molecule 13 is a protein called ATP synthase subunit g, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	g	79	Total	C	H	N	O	S	0	0
			1291	420	662	100	108	1		

- Molecule 14 is a protein called ATP synthase subunit ATP5MPL, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	j	48	Total	C	H	N	O	S	0	0
			828	267	428	66	65	2		

- Molecule 15 is a protein called ATP synthase F(0) complex subunit B1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	b	209	Total	C	H	N	O	S	0	0
			3456	1095	1755	292	308	6		

- Molecule 16 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	h	62	Total	C	H	N	O	S	0	0
			1009	326	495	87	99	2		

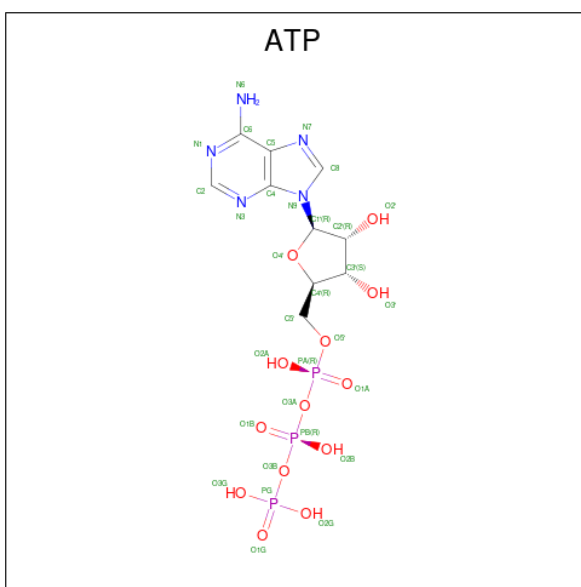
- Molecule 17 is a protein called ATP synthase membrane subunit DAPIT, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	k	36	Total	C	H	N	O	S	0	0
			596	192	307	47	48	2		

- Molecule 18 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	e	56	Total	C	H	N	O	S	0	0
			951	295	487	87	81	1		

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

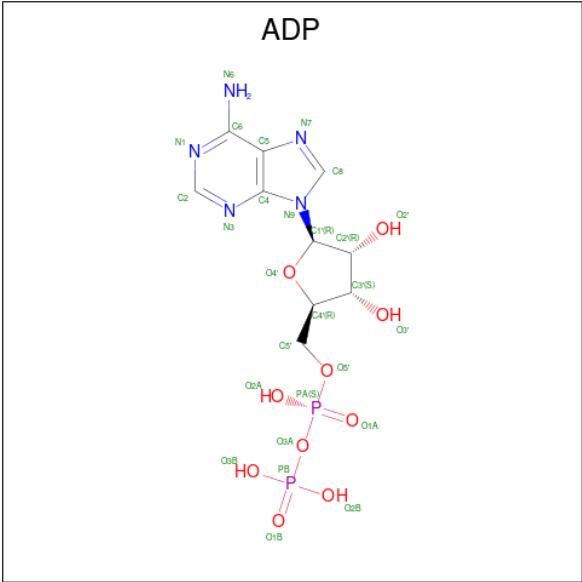


Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
19	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
19	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

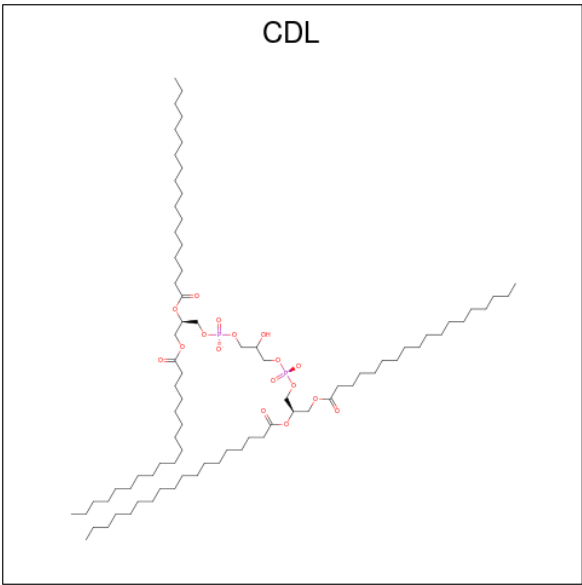
Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total Mg 1 1	0
20	B	1	Total Mg 1 1	0
20	C	1	Total Mg 1 1	0
20	D	1	Total Mg 1 1	0
20	F	1	Total Mg 1 1	0

- Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms						AltConf
21	D	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
21	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
21	F	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



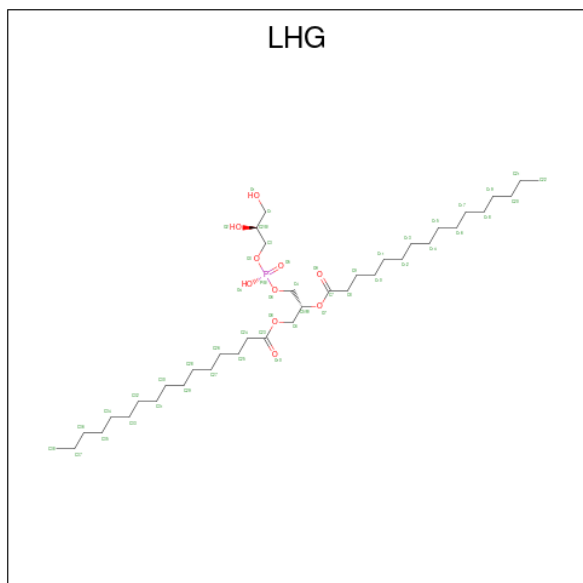
Mol	Chain	Residues	Atoms					AltConf
22	f	1	Total	C	H	O	P	0
			185	65	101	17	2	

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Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	H	O	P	0
			171	59	93	17	2	
22	b	1	Total	C	H	O	P	0
			190	64	107	17	2	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
23	f	1	Total	C	H	O	P	0
			87	28	48	10	1	
23	f	1	Total	C	H	O	P	0
			123	38	74	10	1	

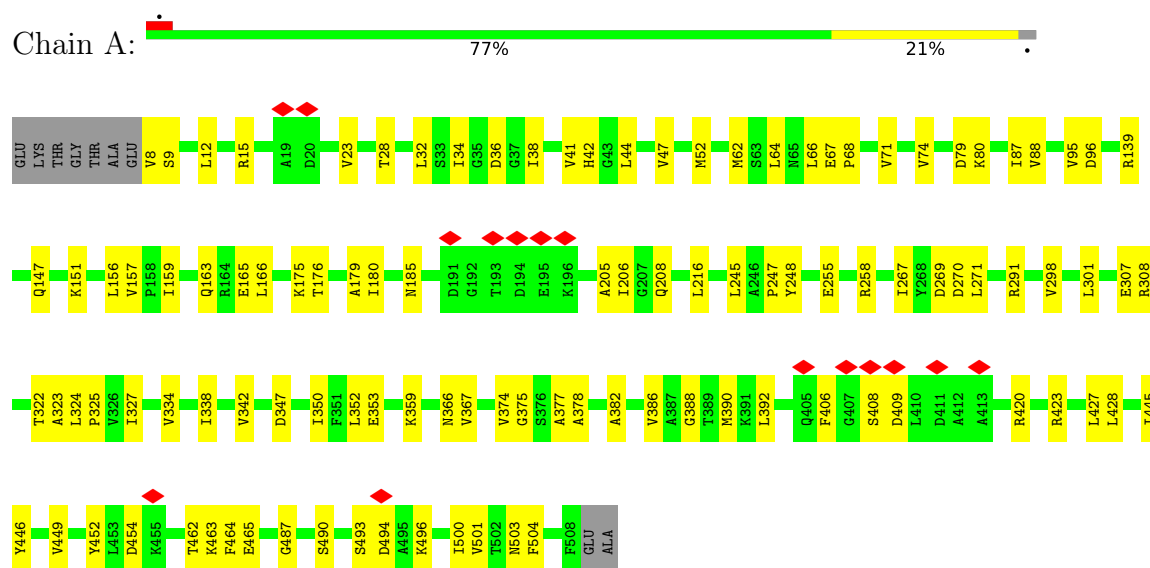
- Molecule 24 is water.

Mol	Chain	Residues	Atoms		AltConf
24	A	3	Total	O	0
			3	3	
24	B	3	Total	O	0
			3	3	
24	C	3	Total	O	0
			3	3	
24	D	4	Total	O	0
			4	4	
24	F	4	Total	O	0
			4	4	

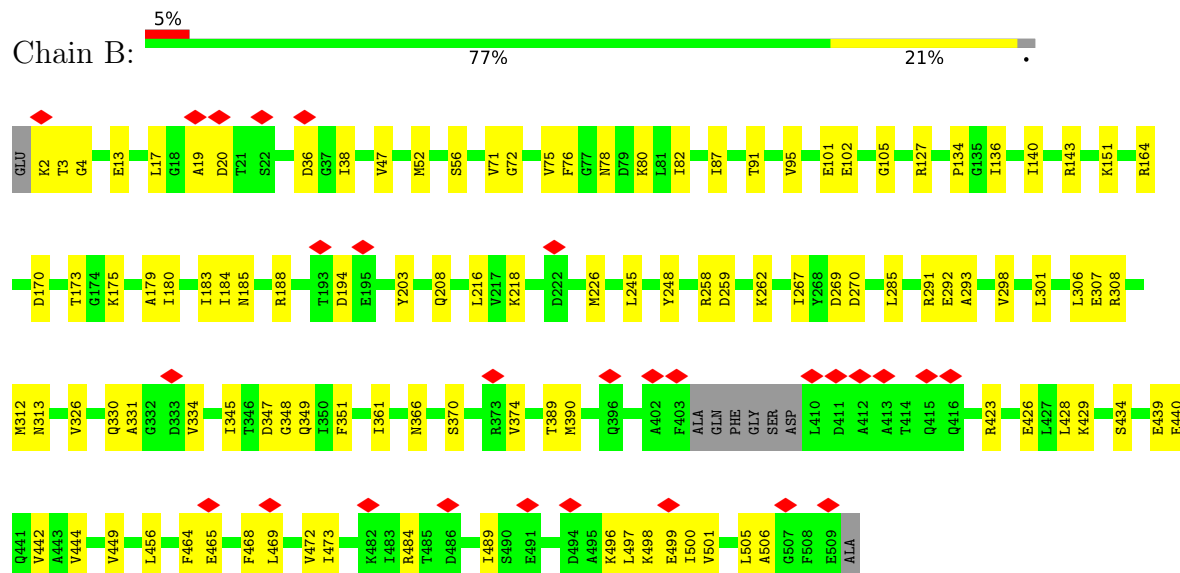
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

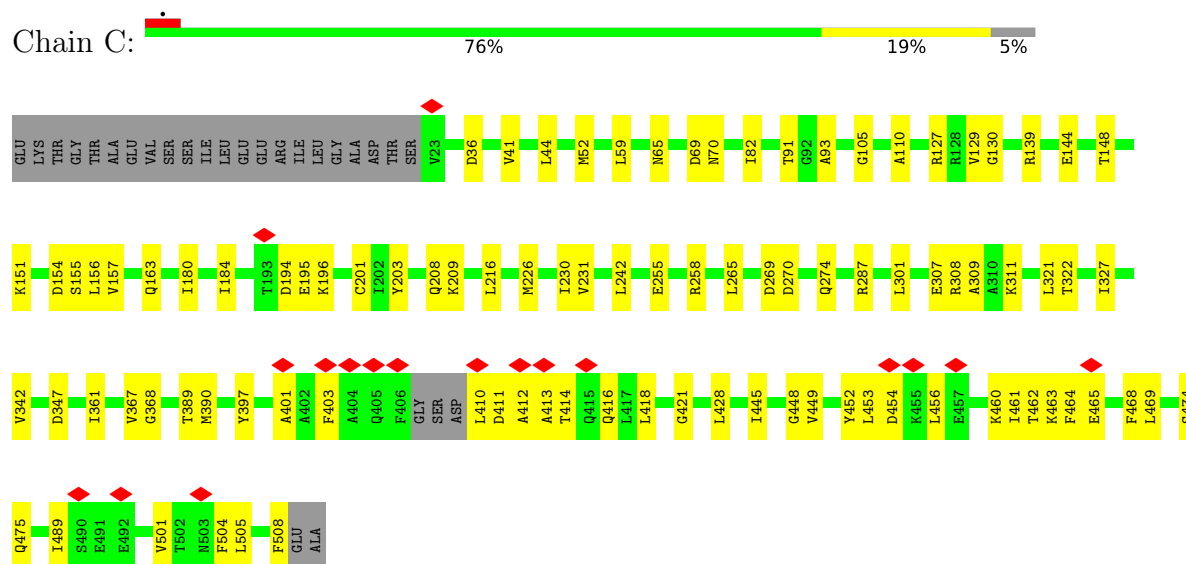
- Molecule 1: ATP synthase subunit alpha, mitochondrial



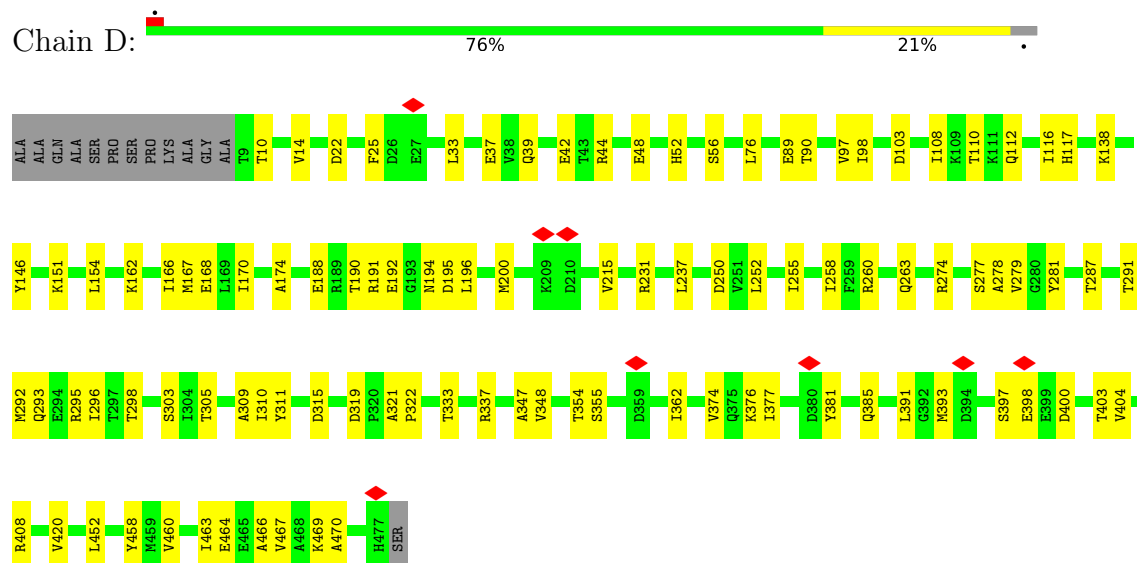
- Molecule 1: ATP synthase subunit alpha, mitochondrial



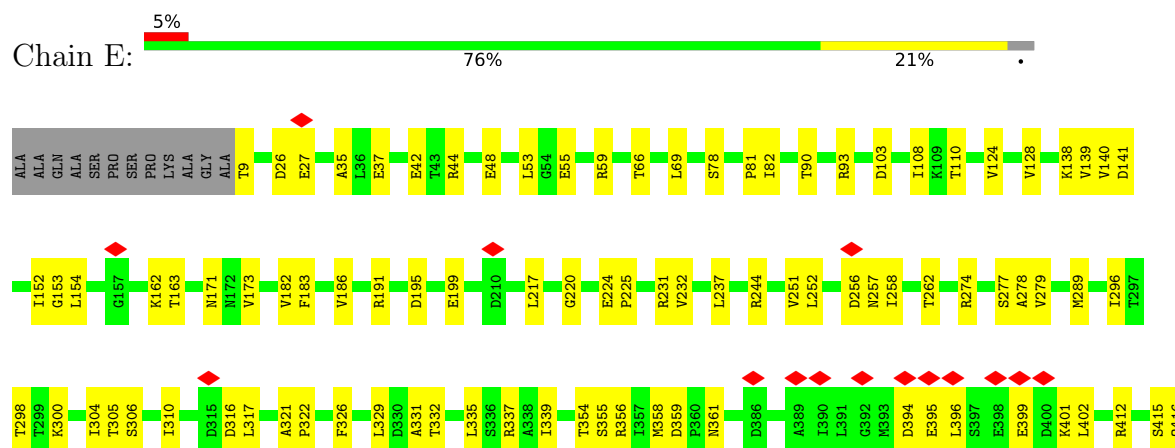
- Molecule 1: ATP synthase subunit alpha, mitochondrial

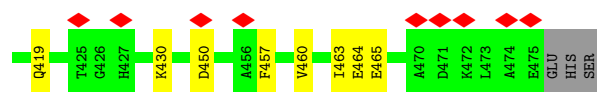


- Molecule 2: ATP synthase subunit beta, mitochondrial



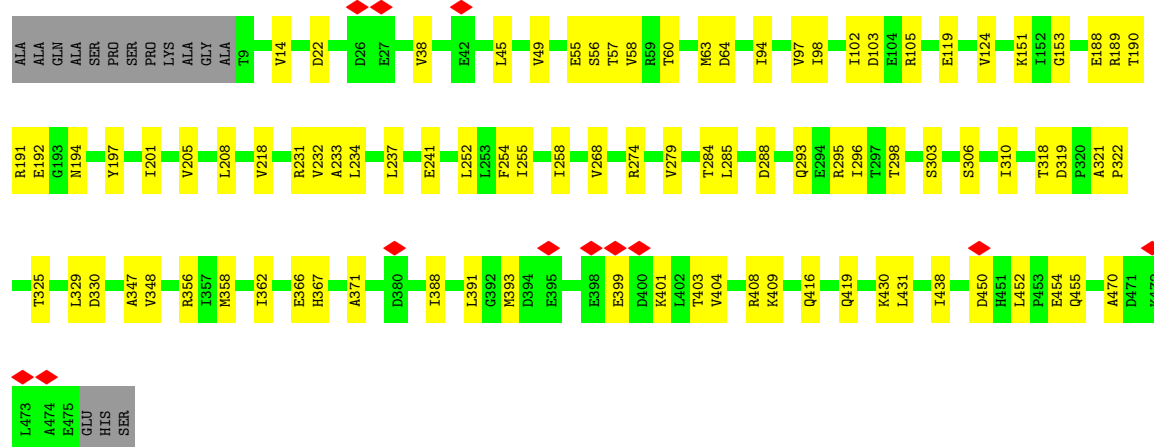
- Molecule 2: ATP synthase subunit beta, mitochondrial





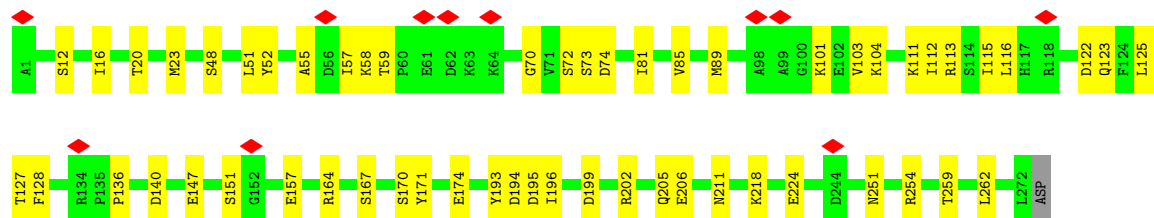
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain F: 78% 19%



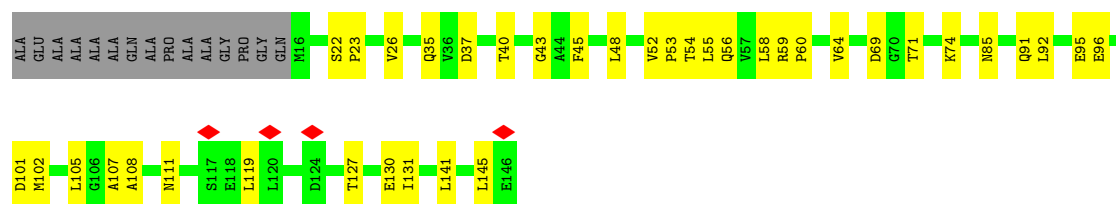
- Molecule 3: ATP synthase subunit gamma, mitochondrial

Chain G: 79% 21%



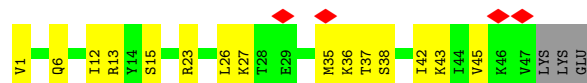
- Molecule 4: ATP synthase subunit delta, mitochondrial

Chain H: 64% 26% 10%

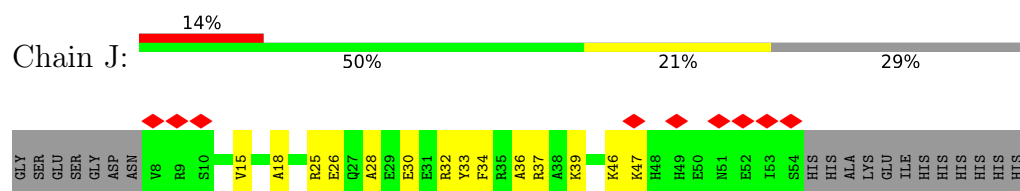


- Molecule 5: ATP synthase subunit epsilon, mitochondrial

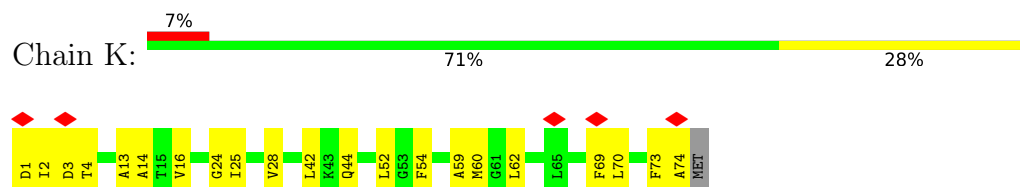
Chain I: 8% 64% 30% 6%



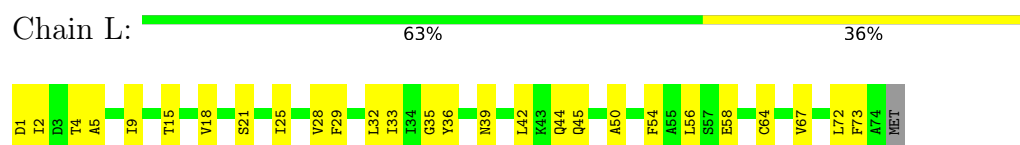
- Molecule 6: ATPase inhibitor, mitochondrial



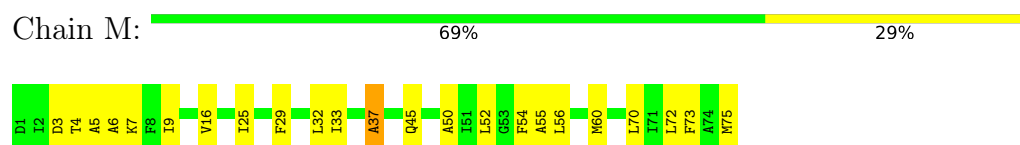
- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial



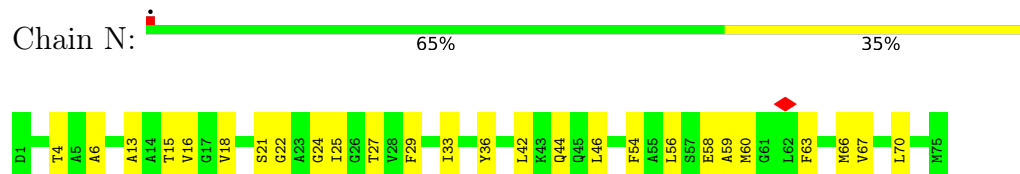
- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial



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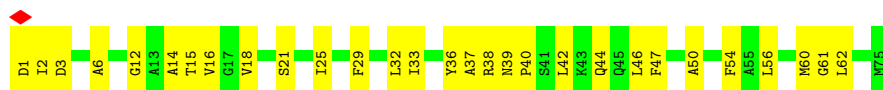


- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial

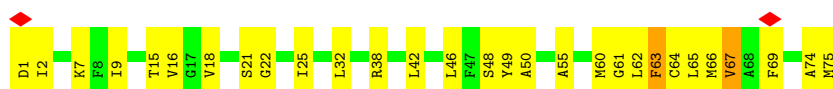




- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial



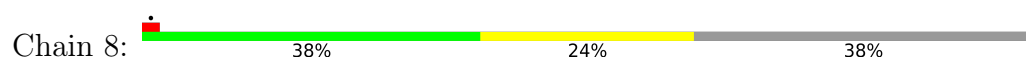
- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial



- Molecule 8: ATP synthase subunit O, mitochondrial



- Molecule 9: ATP synthase protein 8



- Molecule 10: ATP synthase subunit a





- Molecule 11: ATP synthase subunit d, mitochondrial



- Molecule 12: ATP synthase subunit f, mitochondrial



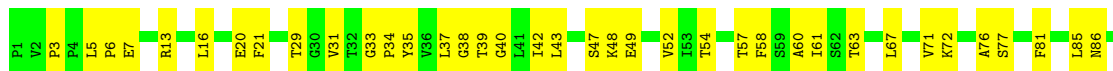
- Molecule 13: ATP synthase subunit g, mitochondrial



- Molecule 14: ATP synthase subunit ATP5MPL, mitochondrial

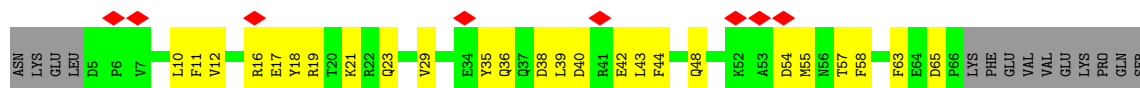


- Molecule 15: ATP synthase F(0) complex subunit B1, mitochondrial

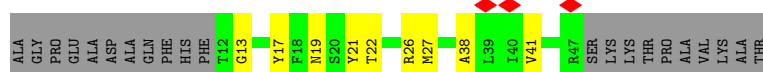




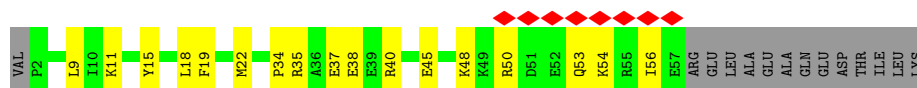
- Molecule 16: ATP synthase-coupling factor 6, mitochondrial



- Molecule 17: ATP synthase membrane subunit DAPIT, mitochondrial



- Molecule 18: ATP synthase subunit e, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61458	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	4.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	45.029	Depositor
Minimum map value	-26.424	Depositor
Average map value	0.017	Depositor
Map value standard deviation	1.103	Depositor
Recommended contour level	7.92	Depositor
Map size (Å)	524.0, 524.0, 524.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, ATP, MG, ADP, CDL, M3L

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.33	0/3869	0.37	0/5220
1	B	0.34	0/3874	0.36	0/5225
1	C	0.34	0/3740	0.38	0/5044
2	D	0.34	0/3616	0.36	0/4906
2	E	0.33	0/3596	0.36	0/4879
2	F	0.34	0/3596	0.37	0/4879
3	G	0.31	0/2141	0.39	0/2876
4	H	0.35	0/982	0.41	0/1337
5	I	0.30	0/374	0.38	0/501
6	J	0.30	0/374	0.49	0/495
7	K	0.36	0/526	0.45	0/711
7	L	0.37	0/526	0.50	0/711
7	M	0.36	0/534	0.53	1/721 (0.1%)
7	N	0.30	0/534	0.48	0/721
7	O	0.41	0/534	0.78	3/721 (0.4%)
7	P	0.87	2/526 (0.4%)	0.73	1/711 (0.1%)
7	Q	0.31	0/534	0.80	5/721 (0.7%)
7	R	0.37	0/534	0.51	0/721
8	S	0.22	0/1455	0.36	0/1957
9	8	0.62	0/355	0.90	0/483
10	a	0.40	0/1779	0.51	0/2433
11	d	0.22	0/1304	0.37	0/1768
12	f	0.31	0/711	0.41	0/952
13	g	0.24	0/646	0.48	0/879
14	j	0.23	0/410	0.37	0/552
15	b	0.25	0/1733	0.40	0/2334
16	h	0.22	0/526	0.48	0/707
17	k	0.18	0/294	0.32	0/395
18	e	0.27	0/472	0.54	0/628
All	All	0.34	2/40095 (0.0%)	0.43	10/54188 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	47	PHE	C-O	-15.16	1.06	1.24
7	P	47	PHE	C-N	-6.75	1.25	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q	63	PHE	N-CA-C	-7.80	102.72	111.14
7	Q	50	ALA	N-CA-C	-7.72	102.80	111.14
7	O	38	ARG	N-CA-C	7.52	120.54	111.82
7	O	37	ALA	N-CA-C	6.71	119.45	111.33
7	O	46	LEU	N-CA-C	-6.19	104.53	111.28
7	P	47	PHE	N-CA-C	-6.13	104.29	110.97
7	Q	50	ALA	N-CA-CB	5.54	118.11	110.07
7	Q	67	VAL	N-CA-C	-5.33	105.34	110.72
7	M	37	ALA	N-CA-C	-5.17	105.64	111.28
7	Q	48	SER	N-CA-C	5.08	117.21	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3818	3923	3924	77	0
1	B	3825	3935	3936	81	0
1	C	3690	3798	3799	76	0
2	D	3558	3605	3605	77	0
2	E	3539	3593	3593	74	0
2	F	3539	3592	3592	68	0
3	G	2115	2185	2185	45	0
4	H	970	970	970	35	0
5	I	369	395	395	14	0
6	J	370	361	361	21	0
7	K	529	550	549	23	0
7	L	529	550	550	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	537	558	559	25	0
7	N	537	559	559	33	0
7	O	537	559	559	39	0
7	P	529	550	548	52	0
7	Q	537	559	559	77	0
7	R	537	559	559	49	0
8	S	1438	1551	1551	46	0
9	8	344	352	352	20	0
10	a	1741	1870	1870	98	0
11	d	1273	1276	1275	75	0
12	f	693	718	718	32	0
13	g	629	662	662	30	0
14	j	400	428	428	13	0
15	b	1701	1755	1755	116	0
16	h	514	495	495	35	0
17	k	289	307	307	6	0
18	e	464	487	487	19	0
19	A	31	12	12	0	0
19	B	31	12	12	2	0
19	C	31	12	12	1	0
20	A	1	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	D	1	0	0	0	0
20	F	1	0	0	0	0
21	D	27	12	12	1	0
21	E	27	12	12	2	0
21	F	27	12	12	0	0
22	b	161	200	216	6	0
22	f	84	101	115	4	0
23	f	88	122	122	2	0
24	A	3	0	0	0	0
24	B	3	0	0	2	0
24	C	3	0	0	1	0
24	D	4	0	0	2	0
24	F	4	0	0	4	0
All	All	40080	41197	41227	1114	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:64:CYS:SG	7:Q:18:VAL:HG21	1.75	1.26
7:R:64:CYS:SG	7:Q:18:VAL:CG2	2.35	1.14
7:R:2:ILE:HD11	7:Q:2:ILE:HG22	1.27	1.14
7:P:58:GLU:OE1	7:Q:60:MET:HE1	1.50	1.09
7:R:2:ILE:CD1	7:Q:2:ILE:HG22	1.81	1.09
7:P:58:GLU:OE1	7:Q:60:MET:CE	2.08	1.00
13:g:38:VAL:O	18:e:11:LYS:NZ	1.93	1.00
3:G:195:ASP:OD2	4:H:56:GLN:NE2	1.95	1.00
7:R:60:MET:HE3	7:Q:22:GLY:N	1.80	0.96
11:d:19:ILE:O	11:d:21:ARG:NH2	1.99	0.96
9:8:31:HIS:ND1	10:a:47:GLN:OE1	2.00	0.94
7:K:60:MET:SD	7:R:21:SER:OG	2.27	0.93
1:B:291:ARG:NH2	2:F:319:ASP:OD1	2.02	0.92
7:R:60:MET:CE	7:Q:21:SER:C	2.42	0.92
11:d:156:PRO:O	11:d:159:THR:OG1	1.88	0.91
1:C:307:GLU:OE2	2:D:190:THR:OG1	1.88	0.91
7:P:8:PHE:HZ	7:Q:75:MET:CG	1.84	0.89
2:F:188:GLU:OE2	24:F:701:HOH:O	1.90	0.89
4:H:101:ASP:O	5:I:27:LYS:NZ	2.05	0.89
8:S:137:VAL:O	8:S:140:SER:OG	1.91	0.88
2:E:316:ASP:OD2	3:G:254:ARG:NH1	2.07	0.87
10:a:40:ASN:OD1	10:a:41:ARG:N	2.07	0.87
11:d:131:THR:N	11:d:134:ASP:OD2	2.07	0.87
2:F:151:LYS:NZ	2:F:293:GLN:O	2.08	0.87
1:A:258:ARG:NH1	1:A:308:ARG:O	2.08	0.87
2:D:151:LYS:NZ	2:D:293:GLN:O	2.08	0.87
1:B:52:MET:O	1:B:91:THR:OG1	1.94	0.86
7:K:16:VAL:CG1	7:R:16:VAL:HG22	2.05	0.86
7:P:8:PHE:HZ	7:Q:75:MET:HG2	1.40	0.86
1:C:403:PHE:CE1	6:J:28:ALA:HB1	2.11	0.86
7:P:62:LEU:HD13	10:a:162:ALA:HB3	1.58	0.86
2:D:166:ILE:HD11	2:D:309:ALA:HB2	1.59	0.85
2:F:189:ARG:NH1	24:F:702:HOH:O	2.10	0.84
2:E:278:ALA:O	3:G:259:THR:OG1	1.94	0.84
10:a:36:ARG:NH1	15:b:3:PRO:O	2.10	0.84
14:j:18:THR:OG1	14:j:19:GLN:OE1	1.94	0.84
2:D:188:GLU:OE2	24:D:701:HOH:O	1.94	0.84
7:R:2:ILE:CD1	7:Q:2:ILE:CG2	2.55	0.83
12:f:77:GLU:N	12:f:77:GLU:OE1	2.11	0.83
13:g:92:ILE:HG23	18:e:22:MET:HE1	1.60	0.83
1:B:56:SER:OG	1:B:87:ILE:O	1.95	0.83
1:B:390:MET:HE1	1:B:428:LEU:HD21	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:192:GLU:OE2	24:D:701:HOH:O	1.96	0.83
7:Q:63:PHE:O	7:Q:66:MET:HG2	1.79	0.82
4:H:95:GLU:OE1	5:I:15:SER:OG	1.98	0.82
2:D:167:MET:HE1	2:D:196:LEU:HD12	1.59	0.82
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.12	0.81
4:H:58:LEU:HD11	4:H:92:LEU:HD11	1.62	0.81
7:P:8:PHE:CZ	7:Q:75:MET:CG	2.63	0.81
7:R:60:MET:CE	7:Q:22:GLY:N	2.42	0.81
8:S:155:ASP:OD1	8:S:157:SER:OG	1.98	0.81
1:C:347:ASP:OD2	2:D:191:ARG:NE	2.13	0.81
7:R:2:ILE:HD11	7:Q:2:ILE:CG2	2.11	0.80
10:a:202:LEU:CD2	7:Q:55:ALA:HB1	2.11	0.80
1:A:255:GLU:OE1	1:A:258:ARG:NH2	2.14	0.80
1:C:208:GLN:NE2	24:C:701:HOH:O	2.12	0.80
1:C:255:GLU:OE2	1:C:308:ARG:NE	2.15	0.80
1:C:144:GLU:OE1	1:C:311:LYS:NZ	2.14	0.80
12:f:53:LYS:NZ	15:b:7:GLU:OE2	2.15	0.80
7:R:64:CYS:SG	7:Q:18:VAL:HG23	2.21	0.80
11:d:68:ASP:OD1	11:d:72:LYS:NZ	2.15	0.80
4:H:130:GLU:OE2	5:I:13:ARG:NH2	2.15	0.79
10:a:1:MET:CE	7:Q:74:ALA:HB2	2.13	0.79
7:R:60:MET:HE1	7:Q:21:SER:C	2.07	0.79
7:R:60:MET:CE	7:Q:21:SER:OG	2.30	0.79
2:E:257:ASN:OD1	2:E:258:ILE:N	2.16	0.79
7:P:56:LEU:HD12	7:O:29:PHE:HE2	1.47	0.79
5:I:36:LYS:O	5:I:37:THR:OG1	2.01	0.79
1:C:151:LYS:NZ	1:C:465:GLU:OE1	2.15	0.79
1:B:258:ARG:NH1	1:B:308:ARG:O	2.15	0.78
1:B:102:GLU:N	1:B:102:GLU:OE1	2.17	0.78
1:C:416:GLN:NE2	1:C:454:ASP:OD2	2.16	0.78
1:A:359:LYS:O	2:D:376:LYS:NZ	2.17	0.78
13:g:92:ILE:CG2	18:e:22:MET:HE1	2.14	0.78
2:E:416:GLN:NE2	2:E:430:LYS:O	2.15	0.78
3:G:136:PRO:O	3:G:218:LYS:NZ	2.17	0.78
1:A:390:MET:HE1	1:A:428:LEU:HD21	1.65	0.77
15:b:143:ARG:NH2	16:h:65:ASP:OD1	2.17	0.77
10:a:129:LEU:O	17:k:26:ARG:NH1	2.17	0.77
7:M:32:LEU:HD12	7:M:50:ALA:HB2	1.67	0.77
7:P:8:PHE:HE2	7:Q:7:LYS:HD3	1.48	0.77
10:a:103:GLY:HA2	14:j:31:MET:HE1	1.67	0.77
22:b:302:CDL:OA4	22:b:302:CDL:O1	2.03	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLU:OE2	1:B:262:LYS:NZ	2.18	0.77
1:A:180:ILE:CD1	1:A:216:LEU:HD11	2.15	0.76
12:f:42:TYR:OH	22:f:101:CDL:OA3	2.01	0.76
13:g:66:GLN:N	13:g:66:GLN:OE1	2.17	0.76
11:d:133:GLU:N	11:d:133:GLU:OE1	2.18	0.76
13:g:48:ALA:O	13:g:51:SER:OG	2.03	0.76
1:B:164:ARG:NH1	1:B:306:LEU:O	2.20	0.75
10:a:184:ILE:HG22	10:a:185:SER:H	1.51	0.75
13:g:71:GLU:OE2	13:g:75:ASN:ND2	2.19	0.75
1:B:347:ASP:OD1	2:F:191:ARG:NE	2.20	0.75
1:A:503:ASN:OD1	1:A:504:PHE:N	2.20	0.75
2:D:200:MET:HE1	2:D:215:VAL:HG11	1.69	0.75
2:D:315:ASP:OD2	2:D:337:ARG:NH2	2.18	0.75
10:a:101:ASN:OD1	10:a:161:THR:OG1	2.04	0.75
1:B:389:THR:HG23	1:B:449:VAL:HG21	1.67	0.74
2:F:409:LYS:NZ	2:F:450:ASP:OD1	2.20	0.74
7:P:8:PHE:CZ	7:Q:75:MET:HG3	2.22	0.74
10:a:199:LEU:HD11	7:Q:62:LEU:HD13	1.68	0.74
7:P:47:PHE:O	7:P:48:SER:C	2.25	0.74
7:P:58:GLU:CD	7:Q:60:MET:HE1	2.12	0.74
7:O:42:LEU:O	7:O:44:GLN:N	2.18	0.74
15:b:154:ARG:NH2	16:h:57:THR:O	2.19	0.74
10:a:1:MET:HE2	7:Q:74:ALA:HB2	1.69	0.74
15:b:154:ARG:HA	16:h:55:MET:HE1	1.68	0.74
2:F:399:GLU:OE1	2:F:399:GLU:N	2.20	0.74
9:8:32:ASN:HB2	11:d:132:ILE:HD12	1.70	0.74
10:a:40:ASN:ND2	12:f:49:VAL:O	2.21	0.74
1:B:52:MET:HE2	1:B:95:VAL:HG23	1.70	0.73
7:P:8:PHE:HE2	7:Q:7:LYS:CD	2.01	0.73
1:B:468:PHE:O	1:B:472:VAL:HG22	1.88	0.73
12:f:16:LEU:HD22	13:g:67:LEU:O	1.88	0.73
7:K:3:ASP:OD1	7:K:4:THR:N	2.22	0.72
1:A:15:ARG:NE	8:S:186:MET:O	2.22	0.72
7:K:42:LEU:O	7:K:44:GLN:N	2.20	0.72
8:S:134:LEU:HD23	15:b:198:ILE:HD13	1.70	0.72
7:N:54:PHE:CE1	7:O:56:LEU:HD23	2.24	0.72
7:R:60:MET:HE2	7:Q:22:GLY:HA2	1.70	0.72
7:M:7:LYS:NZ	7:M:75:MET:O	2.16	0.72
2:D:281:TYR:OH	2:D:319:ASP:OD2	2.05	0.72
2:F:233:ALA:O	2:F:237:LEU:HD23	1.89	0.72
3:G:206:GLU:O	5:I:12:ILE:HD11	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:22:LEU:HD22	8:S:85:LEU:CD2	2.20	0.72
8:S:172:ASP:OD1	8:S:177:THR:HG21	1.89	0.72
1:B:208:GLN:NE2	24:B:702:HOH:O	2.18	0.72
15:b:38:GLY:O	15:b:42:ILE:HD12	1.89	0.72
2:D:458:TYR:O	2:D:469:LYS:NZ	2.23	0.71
7:R:2:ILE:HD13	7:Q:2:ILE:HG22	1.71	0.71
7:O:32:LEU:HD12	7:O:50:ALA:HB2	1.72	0.71
2:F:49:VAL:HA	2:F:60:THR:HG22	1.71	0.71
14:j:14:LYS:O	14:j:18:THR:OG1	2.09	0.71
1:C:180:ILE:HD11	1:C:216:LEU:HD11	1.73	0.71
2:D:166:ILE:CD1	2:D:309:ALA:HB2	2.19	0.71
15:b:169:GLU:OE1	16:h:35:TYR:OH	2.09	0.71
17:k:19:ASN:OD1	17:k:21:TYR:N	2.23	0.71
4:H:69:ASP:OD2	4:H:71:THR:OG1	2.08	0.71
1:B:334:VAL:HG21	1:B:351:PHE:HZ	1.56	0.71
10:a:161:THR:O	10:a:165:THR:HG22	1.90	0.71
15:b:164:MET:SD	15:b:165:MET:N	2.64	0.71
7:P:56:LEU:HD13	7:O:54:PHE:CE1	2.27	0.70
1:B:334:VAL:HG21	1:B:351:PHE:CZ	2.26	0.70
7:P:38:ARG:NH2	7:Q:38:ARG:HD2	2.06	0.70
3:G:51:LEU:CD1	4:H:55:LEU:HD11	2.22	0.70
10:a:73:MET:HE3	10:a:73:MET:HA	1.72	0.70
2:D:255:ILE:HG21	2:D:258:ILE:HD13	1.74	0.70
7:P:58:GLU:CD	7:Q:60:MET:CE	2.64	0.70
2:F:452:LEU:HD22	2:F:470:ALA:HB1	1.75	0.69
12:f:82:ARG:NH1	15:b:49:GLU:OE1	2.23	0.69
1:C:203:TYR:OH	1:C:269:ASP:OD2	2.04	0.69
7:N:13:ALA:O	7:N:16:VAL:HG12	1.92	0.69
15:b:13:ARG:NH1	15:b:35:TYR:OH	2.24	0.69
2:F:408:ARG:NE	2:F:454:GLU:OE2	2.23	0.69
8:S:22:LEU:HD22	8:S:85:LEU:HD22	1.75	0.69
10:a:110:ALA:O	10:a:114:ILE:HG22	1.93	0.69
11:d:130:MET:HE2	11:d:135:LEU:HD22	1.75	0.69
15:b:21:PHE:CD2	22:b:301:CDL:H711	2.28	0.69
12:f:27:ASP:OD2	12:f:28:PHE:N	2.26	0.69
8:S:41:ARG:NH2	8:S:76:GLU:O	2.25	0.69
10:a:119:ASN:OD1	10:a:120:LYS:N	2.26	0.69
7:L:45:GLN:OE1	7:L:45:GLN:N	2.25	0.69
9:8:38:GLU:OE1	9:8:40:THR:N	2.27	0.69
13:g:91:ILE:HD11	15:b:47:SER:CB	2.23	0.68
2:E:171:ASN:ND2	2:E:419:GLN:OE1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:42:LEU:HD12	7:Q:46:LEU:HG	1.74	0.68
10:a:191:ILE:O	10:a:195:ILE:HD12	1.94	0.68
2:D:277:SER:OG	2:D:278:ALA:N	2.24	0.68
4:H:40:THR:O	4:H:59:ARG:NH1	2.26	0.68
15:b:165:MET:SD	15:b:168:LYS:NZ	2.64	0.68
1:A:62:MET:HE2	1:A:64:LEU:HD13	1.73	0.68
1:B:183:ILE:HD11	1:B:267:ILE:HD12	1.74	0.68
19:B:600:ATP:O1G	24:B:701:HOH:O	2.10	0.68
9:8:3:GLN:N	9:8:3:GLN:OE1	2.26	0.67
7:R:60:MET:HA	7:R:63:PHE:HB3	1.77	0.67
2:D:42:GLU:N	2:D:42:GLU:OE1	2.27	0.67
1:A:291:ARG:HA	3:G:262:LEU:HD21	1.74	0.67
2:E:399:GLU:N	2:E:399:GLU:OE1	2.28	0.67
2:E:396:LEU:O	2:E:401:LYS:NZ	2.28	0.67
8:S:15:GLU:N	8:S:15:GLU:OE1	2.27	0.67
10:a:98:LEU:O	10:a:98:LEU:HD23	1.94	0.67
2:E:37:GLU:OE2	2:E:44:ARG:NE	2.24	0.67
7:R:60:MET:HE3	7:Q:21:SER:OG	1.95	0.67
5:I:35:MET:O	5:I:38:SER:OG	2.11	0.66
2:E:163:THR:OG1	21:E:600:ADP:O1A	2.11	0.66
11:d:82:GLU:OE1	11:d:82:GLU:N	2.28	0.66
1:C:403:PHE:CZ	6:J:28:ALA:HB1	2.31	0.66
2:F:279:VAL:HG12	2:F:279:VAL:O	1.96	0.66
3:G:73:SER:OG	3:G:224:GLU:OE2	2.09	0.66
2:D:287:THR:O	2:D:291:THR:HG23	1.95	0.66
11:d:79:PRO:O	15:b:143:ARG:NH1	2.29	0.66
7:Q:61:GLY:O	7:Q:64:CYS:SG	2.46	0.66
1:A:151:LYS:NZ	1:A:427:LEU:O	2.25	0.66
15:b:109:ASP:OD1	15:b:110:MET:N	2.27	0.66
10:a:53:VAL:CG1	10:a:73:MET:HE1	2.26	0.66
13:g:53:LYS:O	13:g:57:ASN:ND2	2.29	0.66
7:P:38:ARG:CZ	7:Q:38:ARG:CD	2.73	0.65
4:H:35:GLN:CD	4:H:48:LEU:HD13	2.21	0.65
4:H:96:GLU:OE1	5:I:23:ARG:NH1	2.28	0.65
7:K:16:VAL:HG13	7:R:16:VAL:HG22	1.79	0.65
1:B:76:PHE:CZ	1:B:245:LEU:HD11	2.32	0.65
7:P:69:PHE:HE2	7:Q:67:VAL:HG22	1.61	0.65
2:D:391:LEU:HG	3:G:23:MET:HE1	1.77	0.65
7:N:25:ILE:HD12	7:N:54:PHE:HD1	1.61	0.65
17:k:13:GLY:O	17:k:17:TYR:N	2.25	0.65
1:C:194:ASP:OD1	1:C:195:GLU:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:42:LEU:O	7:L:44:GLN:N	2.29	0.65
7:P:32:LEU:HD12	7:P:50:ALA:HB2	1.77	0.65
1:B:36:ASP:OD1	2:E:274:ARG:NE	2.30	0.65
2:D:381:TYR:OH	6:J:30:GLU:OE2	2.15	0.65
7:K:13:ALA:O	7:K:16:VAL:HG12	1.97	0.65
7:P:1:ASP:OD1	7:P:2:ILE:N	2.30	0.65
13:g:76:GLY:O	13:g:80:THR:HG23	1.97	0.65
7:Q:62:LEU:HD22	7:Q:65:LEU:HD23	1.77	0.65
1:B:366:ASN:O	1:B:370:SER:OG	2.15	0.64
12:f:8:GLU:N	12:f:8:GLU:OE1	2.31	0.64
3:G:16:ILE:O	3:G:20:THR:HG23	1.97	0.64
1:A:347:ASP:OD2	2:E:191:ARG:NE	2.28	0.64
1:B:426:GLU:OE2	1:B:429:LYS:NZ	2.21	0.64
2:D:258:ILE:HD11	2:D:292:MET:CE	2.28	0.64
4:H:102:MET:O	5:I:26:LEU:HD13	1.98	0.64
1:B:13:GLU:OE2	8:S:28:LYS:NZ	2.20	0.64
1:B:136:ILE:O	2:F:194:ASN:ND2	2.31	0.64
12:f:52:LYS:NZ	15:b:5:LEU:O	2.30	0.64
7:R:1:ASP:OD1	7:R:2:ILE:N	2.31	0.64
2:D:168:GLU:OE2	2:D:420:VAL:HG13	1.97	0.64
11:d:131:THR:O	11:d:134:ASP:N	2.30	0.64
11:d:22:ASN:OD1	11:d:23:GLN:N	2.32	0.63
2:F:55:GLU:O	2:F:56:SER:OG	2.16	0.63
2:F:284:THR:OG1	2:F:288:ASP:OD2	2.14	0.63
7:N:60:MET:N	7:N:60:MET:HE2	2.14	0.63
9:8:6:THR:O	14:j:39:ARG:NH2	2.31	0.63
15:b:110:MET:O	15:b:113:SER:OG	2.14	0.63
1:C:52:MET:O	1:C:91:THR:HG22	1.97	0.63
8:S:186:MET:SD	15:b:174:ILE:HD12	2.38	0.63
16:h:36:GLN:N	16:h:36:GLN:OE1	2.30	0.63
7:M:32:LEU:HD12	7:M:50:ALA:CB	2.28	0.63
7:N:25:ILE:HD12	7:N:54:PHE:CD1	2.34	0.63
15:b:49:GLU:OE2	15:b:52:VAL:HG12	1.99	0.63
22:f:101:CDL:OB3	22:f:101:CDL:O1	2.16	0.62
12:f:52:LYS:NZ	15:b:6:PRO:O	2.29	0.62
7:K:69:PHE:O	7:K:73:PHE:N	2.32	0.62
7:R:16:VAL:HG12	7:R:16:VAL:O	1.99	0.62
12:f:16:LEU:HD21	13:g:65:LYS:O	1.98	0.62
1:A:66:LEU:HD23	1:A:71:VAL:HG23	1.81	0.62
2:E:277:SER:OG	2:E:278:ALA:N	2.32	0.62
3:G:51:LEU:HD13	4:H:55:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LYS:HG2	1:A:352:LEU:HD12	1.81	0.62
2:F:367:HIS:CD2	2:F:438:ILE:HD11	2.34	0.62
12:f:61:MET:HE2	12:f:61:MET:HA	1.81	0.62
2:F:231:ARG:O	2:F:234:LEU:N	2.33	0.62
7:L:32:LEU:HD12	7:L:50:ALA:HB2	1.81	0.62
9:8:38:GLU:C	9:8:39:LEU:HD12	2.24	0.62
1:B:496:LYS:O	1:B:500:ILE:HD12	2.00	0.62
16:h:21:LYS:NZ	16:h:29:VAL:HG12	2.15	0.62
1:B:3:THR:HG22	1:B:4:GLY:H	1.65	0.62
7:O:1:ASP:OD1	7:O:2:ILE:N	2.33	0.62
2:E:173:VAL:HG21	2:E:252:LEU:HD21	1.82	0.61
5:I:1:VAL:O	5:I:6:GLN:NE2	2.33	0.61
7:L:64:CYS:O	7:L:67:VAL:HG12	2.00	0.61
7:K:16:VAL:CG1	7:R:16:VAL:CG2	2.78	0.61
2:F:399:GLU:O	2:F:403:THR:HG23	1.99	0.61
3:G:194:ASP:OD1	3:G:195:ASP:N	2.33	0.61
11:d:40:ARG:HH21	15:b:138:VAL:HG22	1.65	0.61
2:F:63:MET:HE1	2:F:231:ARG:HG3	1.82	0.61
15:b:29:THR:HG21	15:b:33:GLY:HA3	1.82	0.61
1:C:59:LEU:HD12	1:C:82:ILE:HD11	1.82	0.61
13:g:91:ILE:HD11	15:b:47:SER:HB3	1.82	0.61
2:E:279:VAL:HG12	2:E:279:VAL:O	2.01	0.61
7:N:44:GLN:O	7:N:44:GLN:NE2	2.33	0.61
2:E:220:GLY:N	2:E:232:VAL:HG21	2.16	0.60
7:P:58:GLU:OE1	7:Q:60:MET:HE3	1.96	0.60
11:d:18:ILE:HG23	11:d:19:ILE:N	2.16	0.60
2:F:188:GLU:OE2	24:F:703:HOH:O	2.16	0.60
11:d:131:THR:OG1	11:d:134:ASP:OD2	2.13	0.60
7:P:55:ALA:HB2	10:a:213:VAL:CG2	2.31	0.60
2:E:430:LYS:NZ	2:E:465:GLU:OE2	2.34	0.60
7:N:16:VAL:CG2	7:O:16:VAL:HG13	2.31	0.60
7:R:60:MET:HE1	7:Q:21:SER:CB	2.31	0.60
8:S:118:CYS:SG	8:S:119:THR:N	2.74	0.60
1:C:110:ALA:HB3	1:C:242:LEU:HD22	1.84	0.60
4:H:64:VAL:HG12	4:H:74:LYS:HG2	1.84	0.60
1:C:411:ASP:OD1	1:C:412:ALA:N	2.34	0.60
2:D:138:LYS:NZ	2:D:460:VAL:O	2.35	0.60
7:R:2:ILE:HD13	7:Q:2:ILE:CG2	2.29	0.60
2:D:237:LEU:HD21	2:D:295:ARG:HB2	1.84	0.60
1:B:423:ARG:NH2	1:B:456:LEU:O	2.35	0.60
15:b:115:GLN:O	15:b:119:GLN:NE2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:LEU:O	1:B:505:LEU:HD23	2.02	0.59
7:R:60:MET:CE	7:Q:21:SER:HG	2.13	0.59
1:B:440:GLU:OE2	1:B:473:ILE:HD11	2.01	0.59
7:M:54:PHE:CE1	7:N:56:LEU:HD21	2.37	0.59
15:b:154:ARG:NH1	16:h:54:ASP:O	2.35	0.59
15:b:157:TYR:CB	16:h:55:MET:HE2	2.32	0.59
2:E:183:PHE:HB3	2:E:217:LEU:HD23	1.83	0.59
2:F:391:LEU:HD11	6:J:25:ARG:NH1	2.18	0.59
1:A:390:MET:HE1	1:A:428:LEU:CD2	2.32	0.59
10:a:86:GLY:O	10:a:91:SER:OG	2.20	0.59
2:D:33:LEU:HD13	2:D:117:HIS:CG	2.36	0.59
15:b:101:ILE:O	15:b:105:GLN:NE2	2.35	0.59
2:E:298:THR:HG23	2:E:298:THR:O	2.03	0.59
18:e:50:ARG:NH2	18:e:53:GLN:OE1	2.35	0.59
1:A:166:LEU:HD11	1:A:327:ILE:HG13	1.84	0.59
1:B:465:GLU:O	1:B:469:LEU:HD23	2.03	0.59
7:P:8:PHE:CD2	7:Q:7:LYS:HG2	2.38	0.59
1:B:127:ARG:NH2	1:B:259:ASP:OD2	2.36	0.58
8:S:137:VAL:HG11	15:b:198:ILE:HD11	1.84	0.58
10:a:100:MET:HE2	10:a:104:MET:CE	2.33	0.58
11:d:110:ARG:NH2	15:b:111:GLU:OE2	2.36	0.58
4:H:127:THR:O	4:H:131:ILE:HD12	2.02	0.58
12:f:78:LEU:HD12	12:f:78:LEU:O	2.02	0.58
15:b:134:MET:O	15:b:138:VAL:HG23	2.02	0.58
1:B:2:LYS:O	1:B:3:THR:OG1	2.16	0.58
1:B:75:VAL:HG11	1:B:82:ILE:HD13	1.86	0.58
2:E:354:THR:HG22	2:E:355:SER:N	2.19	0.58
7:L:1:ASP:OD1	7:L:2:ILE:N	2.35	0.58
7:P:8:PHE:CZ	7:Q:75:MET:HG2	2.29	0.58
1:A:180:ILE:HD12	1:A:216:LEU:HD11	1.85	0.58
2:E:93:ARG:NE	2:E:103:ASP:OD2	2.33	0.58
2:E:310:ILE:CD1	2:E:329:LEU:HD11	2.34	0.58
10:a:15:LEU:O	10:a:17:LEU:N	2.36	0.58
3:G:122:ASP:OD1	3:G:123:GLN:N	2.37	0.57
7:O:39:ASN:CG	7:O:42:LEU:HD13	2.28	0.57
1:C:448:GLY:HA2	1:C:453:LEU:HD12	1.86	0.57
11:d:131:THR:OG1	11:d:133:GLU:OE2	2.21	0.57
1:C:452:TYR:HD1	1:C:501:VAL:HG11	1.68	0.57
1:B:134:PRO:HB3	1:B:312:MET:HE1	1.85	0.57
1:C:157:VAL:HG13	1:C:157:VAL:O	2.05	0.57
11:d:15:PHE:O	11:d:18:ILE:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:THR:HG23	1:A:87:ILE:HG23	1.87	0.57
2:F:268:VAL:HG22	2:F:268:VAL:O	2.03	0.57
7:R:14:ALA:HB1	7:Q:15:THR:HG21	1.87	0.57
8:S:182:LEU:HD21	16:h:10:LEU:HD13	1.86	0.57
2:D:90:THR:HG22	2:D:108:ILE:HG21	1.85	0.57
10:a:202:LEU:HD21	7:Q:55:ALA:HB1	1.84	0.57
1:A:322:THR:HG22	1:A:323:ALA:N	2.21	0.56
1:C:201:CYS:SG	1:C:265:LEU:HD23	2.45	0.56
3:G:199:ASP:OD1	3:G:202:ARG:NH1	2.38	0.56
8:S:127:ASP:OD2	8:S:129:ALA:N	2.37	0.56
10:a:107:PRO:HG3	14:j:31:MET:HE3	1.86	0.56
10:a:44:THR:HG21	15:b:86:ASN:OD1	2.05	0.56
11:d:19:ILE:HG21	11:d:24:LYS:HA	1.87	0.56
2:E:359:ASP:OD2	2:E:361:ASN:ND2	2.39	0.56
10:a:29:LEU:HD23	22:f:101:CDL:H732	1.86	0.56
7:Q:1:ASP:OD1	7:Q:2:ILE:N	2.39	0.56
1:A:38:ILE:CD1	1:A:74:VAL:HG12	2.36	0.56
7:R:60:MET:CE	7:Q:22:GLY:CA	2.83	0.56
7:O:39:ASN:ND2	7:O:42:LEU:HD13	2.20	0.56
22:f:101:CDL:OA4	14:j:8:LYS:NZ	2.38	0.56
4:H:35:GLN:HE22	4:H:48:LEU:HD22	1.70	0.56
7:M:16:VAL:CG2	7:N:16:VAL:HG13	2.36	0.56
2:D:464:GLU:O	2:D:467:VAL:HG22	2.05	0.56
2:F:38:VAL:HG21	2:F:45:LEU:HD23	1.86	0.56
7:M:45:GLN:N	7:M:45:GLN:OE1	2.38	0.56
13:g:32:TYR:CD1	15:b:31:VAL:HG21	2.40	0.56
15:b:154:ARG:CA	16:h:55:MET:HE1	2.36	0.56
13:g:84:MET:HE1	15:b:40:GLY:HA3	1.88	0.56
1:B:439:GLU:OE2	1:B:484:ARG:NE	2.38	0.56
10:a:53:VAL:HG12	10:a:73:MET:HE1	1.87	0.56
7:P:56:LEU:HD12	7:O:29:PHE:CE2	2.34	0.56
1:A:423:ARG:NH2	1:A:454:ASP:O	2.39	0.55
1:C:180:ILE:CD1	1:C:216:LEU:HD11	2.36	0.55
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.36	0.55
10:a:199:LEU:HD11	7:Q:62:LEU:CD1	2.36	0.55
7:N:4:THR:OG1	7:O:3:ASP:OD1	2.11	0.55
2:D:48:GLU:OE1	2:D:231:ARG:NE	2.40	0.55
15:b:173:MET:HE1	16:h:21:LYS:NZ	2.22	0.55
2:D:200:MET:CE	2:D:215:VAL:HG11	2.36	0.55
11:d:18:ILE:HD11	15:b:121:ARG:HD2	1.87	0.55
7:R:60:MET:CE	7:Q:22:GLY:HA2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LYS:HE2	2:D:33:LEU:HD12	1.87	0.55
7:K:25:ILE:HD12	7:K:54:PHE:CD2	2.42	0.55
2:D:89:GLU:HB2	2:D:110:THR:HG22	1.89	0.55
2:F:358:MET:HE1	2:F:371:ALA:HB3	1.87	0.55
11:d:56:TYR:CD2	15:b:155:LEU:HD13	2.42	0.55
2:D:408:ARG:NH1	6:J:30:GLU:OE2	2.36	0.55
7:P:33:ILE:CD1	7:Q:49:TYR:HB2	2.37	0.55
1:B:164:ARG:NH2	1:B:345:ILE:O	2.40	0.55
2:E:251:VAL:HG12	2:E:252:LEU:O	2.07	0.55
7:P:33:ILE:HD11	7:Q:49:TYR:HB2	1.89	0.55
10:a:195:ILE:O	10:a:199:LEU:HD23	2.06	0.55
1:A:52:MET:HG2	1:A:95:VAL:HG22	1.88	0.54
1:C:127:ARG:NH2	1:C:255:GLU:OE1	2.38	0.54
7:R:42:LEU:O	7:R:44:GLN:N	2.33	0.54
1:A:322:THR:HG22	1:A:323:ALA:H	1.73	0.54
18:e:34:PRO:O	18:e:38:GLU:OE1	2.25	0.54
7:K:70:LEU:O	7:K:74:ALA:N	2.41	0.54
7:L:15:THR:O	7:L:18:VAL:HG12	2.06	0.54
9:8:32:ASN:CG	9:8:33:PHE:N	2.65	0.54
1:B:444:VAL:HG11	1:B:469:LEU:HD21	1.89	0.54
13:g:91:ILE:HD11	15:b:47:SER:HB2	1.89	0.54
7:L:54:PHE:CZ	7:M:56:LEU:HD11	2.42	0.54
10:a:103:GLY:HA2	14:j:31:MET:CE	2.37	0.54
1:C:410:LEU:HD11	6:J:32:ARG:NH2	2.22	0.54
3:G:167:SER:CB	3:G:170:SER:HG	2.18	0.54
4:H:58:LEU:HD11	4:H:92:LEU:CD1	2.37	0.54
12:f:39:ARG:NH2	23:f:102:LHG:O1	2.37	0.54
10:a:182:MET:HE3	10:a:182:MET:HA	1.90	0.54
2:E:394:ASP:OD1	2:E:395:GLU:N	2.41	0.54
15:b:39:THR:O	15:b:43:LEU:HD23	2.08	0.54
1:A:406:PHE:O	1:A:408:SER:N	2.42	0.53
1:B:134:PRO:CB	1:B:312:MET:HE1	2.37	0.53
7:K:25:ILE:HD12	7:K:54:PHE:HD2	1.73	0.53
7:M:4:THR:HG22	7:M:4:THR:O	2.08	0.53
10:a:202:LEU:HD22	7:Q:55:ALA:HB1	1.91	0.53
1:B:307:GLU:OE2	2:F:190:THR:OG1	2.17	0.53
1:C:403:PHE:CE2	6:J:32:ARG:NH1	2.77	0.53
7:N:54:PHE:CZ	7:O:56:LEU:HD23	2.43	0.53
8:S:186:MET:CE	15:b:174:ILE:HD12	2.39	0.53
12:f:7:LYS:HE2	12:f:7:LYS:HA	1.90	0.53
1:A:180:ILE:HD11	1:A:216:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:21:SER:O	12:f:25:MET:HG3	2.09	0.53
15:b:89:LYS:O	15:b:93:LEU:HD23	2.09	0.53
1:A:41:VAL:HG11	1:A:44:LEU:HD12	1.90	0.53
4:H:40:THR:OG1	4:H:43:GLY:O	2.26	0.53
10:a:80:GLY:O	10:a:84:LEU:HD23	2.09	0.53
15:b:47:SER:OG	15:b:48:LYS:N	2.39	0.53
1:B:334:VAL:HG22	1:B:334:VAL:O	2.07	0.53
1:B:140:ILE:HD12	1:B:143:ARG:HE	1.74	0.53
1:C:209:LYS:NZ	2:F:330:ASP:OD1	2.26	0.53
3:G:147:GLU:O	3:G:151:SER:OG	2.24	0.53
8:S:62:ARG:NH1	8:S:91:GLU:O	2.41	0.53
13:g:97:ILE:HD12	13:g:97:ILE:H	1.74	0.53
1:B:3:THR:HG22	1:B:4:GLY:N	2.24	0.53
1:C:456:LEU:HD21	1:C:505:LEU:HD11	1.90	0.53
1:C:194:ASP:OD1	1:C:196:LYS:N	2.40	0.52
2:D:258:ILE:HD11	2:D:292:MET:HE2	1.89	0.52
2:E:262:THR:CG2	2:E:289:MET:HE1	2.39	0.52
11:d:118:LEU:C	11:d:118:LEU:HD23	2.34	0.52
16:h:38:ASP:O	16:h:42:GLU:HG3	2.09	0.52
1:C:65:ASN:OD1	1:C:287:ARG:NH2	2.40	0.52
11:d:93:GLU:OE1	11:d:93:GLU:N	2.41	0.52
2:F:241:GLU:OE1	2:F:295:ARG:NH2	2.37	0.52
7:P:32:LEU:C	7:P:32:LEU:HD23	2.34	0.52
10:a:184:ILE:HG22	10:a:185:SER:N	2.23	0.52
11:d:91:ALA:HB1	15:b:125:PHE:CZ	2.44	0.52
12:f:51:VAL:HG12	15:b:6:PRO:HB2	1.90	0.52
16:h:10:LEU:HD12	16:h:11:PHE:N	2.24	0.52
13:g:97:ILE:O	13:g:97:ILE:HG22	2.10	0.52
1:B:151:LYS:NZ	1:B:465:GLU:OE2	2.41	0.52
11:d:89:VAL:N	15:b:129:ARG:NH1	2.58	0.52
2:E:124:VAL:O	2:E:300:LYS:NZ	2.35	0.52
7:P:47:PHE:CZ	7:Q:49:TYR:CE1	2.98	0.52
10:a:19:LEU:HD23	10:a:19:LEU:C	2.34	0.52
15:b:126:ASP:O	15:b:130:ASN:ND2	2.42	0.52
2:D:258:ILE:HD11	2:D:292:MET:HE1	1.90	0.52
7:M:54:PHE:O	7:M:55:ALA:C	2.52	0.52
7:N:36:TYR:CE2	7:O:42:LEU:HD23	2.45	0.52
8:S:65:LYS:O	8:S:69:LEU:HD23	2.09	0.52
11:d:10:ILE:HD13	15:b:127:VAL:HG22	1.91	0.52
11:d:72:LYS:O	11:d:76:LEU:HD23	2.09	0.52
15:b:97:LYS:O	15:b:100:SER:OG	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:105:LEU:HD13	4:H:145:LEU:HB2	1.92	0.52
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.92	0.52
2:D:362:ILE:HG22	2:D:362:ILE:O	2.09	0.52
7:Q:65:LEU:HD11	7:Q:69:PHE:CZ	2.45	0.52
1:B:17:LEU:CD1	1:B:19:ALA:HB2	2.39	0.52
1:C:148:THR:OG1	1:C:154:ASP:OD1	2.25	0.52
2:D:112:GLN:OE1	2:D:112:GLN:N	2.44	0.51
2:F:237:LEU:HD11	2:F:296:ILE:HG13	1.91	0.51
7:M:32:LEU:C	7:M:32:LEU:HD23	2.35	0.51
7:P:8:PHE:CE2	7:Q:7:LYS:HG2	2.45	0.51
10:a:94:PRO:C	10:a:100:MET:SD	2.93	0.51
2:D:146:TYR:OH	2:D:333:THR:HG21	2.11	0.51
2:E:305:THR:HG22	2:E:306:SER:H	1.75	0.51
2:F:197:TYR:CZ	2:F:201:ILE:HD11	2.45	0.51
7:K:52:LEU:C	7:K:52:LEU:HD23	2.35	0.51
2:D:393:MET:HE2	6:J:34:PHE:CE2	2.45	0.51
2:E:9:THR:HG23	2:E:27:GLU:CD	2.36	0.51
1:A:490:SER:O	1:A:493:SER:N	2.44	0.51
2:D:279:VAL:HG12	2:D:279:VAL:O	2.09	0.51
8:S:161:GLY:HA3	8:S:173:MET:O	2.11	0.51
15:b:93:LEU:O	15:b:96:VAL:HG12	2.11	0.51
15:b:169:GLU:O	15:b:173:MET:HG2	2.11	0.51
1:A:420:ARG:NH1	1:A:449:VAL:O	2.44	0.51
2:E:173:VAL:HG11	2:E:252:LEU:HD23	1.92	0.51
11:d:8:LYS:NZ	15:b:130:ASN:OD1	2.43	0.51
1:A:36:ASP:OD1	2:D:274:ARG:NH1	2.44	0.51
2:D:154:LEU:HD23	2:D:333:THR:OG1	2.11	0.51
7:L:29:PHE:O	7:L:33:ILE:HG12	2.11	0.51
7:M:25:ILE:HD12	7:M:54:PHE:CD1	2.46	0.51
10:a:75:LEU:HD11	10:a:79:ILE:HD11	1.91	0.51
11:d:113:GLU:O	11:d:117:GLU:OE1	2.28	0.51
15:b:54:THR:O	15:b:57:THR:N	2.39	0.51
4:H:54:THR:O	4:H:55:LEU:HD22	2.11	0.51
10:a:97:GLN:N	10:a:97:GLN:OE1	2.44	0.51
11:d:37:LEU:HB3	15:b:134:MET:HE1	1.92	0.51
2:D:97:VAL:HG13	2:D:98:ILE:HG23	1.92	0.51
2:E:182:VAL:HG12	2:E:183:PHE:N	2.25	0.51
2:F:318:THR:O	2:F:318:THR:HG22	2.09	0.51
10:a:42:PHE:CE1	12:f:59:LEU:HD13	2.46	0.51
11:d:99:SER:HB2	15:b:118:VAL:HG13	1.93	0.51
13:g:55:ILE:O	13:g:58:SER:OG	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:190:GLU:OE1	15:b:190:GLU:N	2.42	0.51
1:B:330:GLN:O	1:B:331:ALA:C	2.54	0.51
2:D:25:PHE:O	2:D:56:SER:OG	2.25	0.51
3:G:58:LYS:HE2	3:G:58:LYS:HA	1.93	0.51
7:K:62:LEU:HD12	7:K:62:LEU:C	2.36	0.51
11:d:40:ARG:O	11:d:40:ARG:NH1	2.44	0.51
12:f:59:LEU:O	12:f:60:SER:C	2.54	0.51
2:E:66:THR:HB	2:E:69:LEU:HD12	1.93	0.50
8:S:31:LYS:O	8:S:35:VAL:HG23	2.11	0.50
11:d:111:ILE:O	11:d:114:TYR:N	2.44	0.50
12:f:62:VAL:HG23	12:f:63:LEU:HD12	1.93	0.50
18:e:34:PRO:HA	18:e:37:GLU:HG2	1.93	0.50
1:C:403:PHE:CD2	6:J:32:ARG:NH1	2.79	0.50
15:b:174:ILE:HG22	15:b:178:GLU:OE1	2.12	0.50
2:D:37:GLU:OE2	2:D:44:ARG:NE	2.44	0.50
2:E:90:THR:HG22	2:E:108:ILE:HG21	1.92	0.50
7:M:72:LEU:HD23	7:M:73:PHE:CE1	2.46	0.50
7:O:2:ILE:O	7:O:6:ALA:N	2.37	0.50
11:d:86:THR:HA	15:b:129:ARG:NH2	2.27	0.50
11:d:111:ILE:O	11:d:112:GLN:C	2.54	0.50
1:A:41:VAL:CG2	1:A:88:VAL:HG21	2.41	0.50
1:C:389:THR:OG1	1:C:449:VAL:HG21	2.12	0.50
1:C:452:TYR:CD1	1:C:501:VAL:HG11	2.46	0.50
8:S:176:LYS:O	8:S:180:GLN:OE1	2.30	0.50
10:a:89:PRO:HB3	15:b:60:ALA:HB2	1.94	0.50
11:d:93:GLU:O	11:d:96:ASP:HB3	2.12	0.50
2:D:252:LEU:HD23	2:D:305:THR:HB	1.94	0.50
2:D:170:ILE:O	2:D:174:ALA:HB3	2.11	0.50
2:E:152:ILE:H	2:E:152:ILE:HD12	1.77	0.50
2:F:14:VAL:HG12	2:F:22:ASP:O	2.12	0.50
23:f:102:LHG:O5	23:f:102:LHG:O2	2.25	0.50
1:A:95:VAL:HG11	1:A:245:LEU:HD21	1.92	0.50
2:D:168:GLU:OE2	2:D:420:VAL:HG22	2.12	0.50
5:I:23:ARG:HA	5:I:26:LEU:HD23	1.92	0.50
8:S:122:THR:HG21	8:S:126:LEU:HD22	1.93	0.50
10:a:158:VAL:O	10:a:159:ARG:C	2.54	0.50
2:E:457:PHE:HE2	2:E:463:ILE:HD11	1.77	0.49
3:G:52:TYR:OH	3:G:205:GLN:OE1	2.29	0.49
13:g:83:TRP:O	13:g:86:PHE:HB3	2.11	0.49
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.42	0.49
13:g:81:GLU:OE2	15:b:37:LEU:HA	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ASP:OD1	1:C:70:ASN:N	2.45	0.49
7:R:14:ALA:CB	7:Q:15:THR:HG21	2.43	0.49
12:f:43:ARG:NH2	22:b:301:CDL:OA3	2.41	0.49
15:b:20:GLU:CG	22:b:301:CDL:HB62	2.42	0.49
15:b:20:GLU:HG3	22:b:301:CDL:HB62	1.93	0.49
4:H:35:GLN:NE2	4:H:48:LEU:HD13	2.27	0.49
7:L:58:GLU:HA	7:L:58:GLU:OE1	2.12	0.49
7:P:38:ARG:CZ	7:Q:38:ARG:HD2	2.40	0.49
8:S:55:LEU:HD13	8:S:95:LEU:HD12	1.93	0.49
11:d:85:TYR:HB2	15:b:132:ILE:HG21	1.94	0.49
1:A:452:TYR:CD1	1:A:501:VAL:HG11	2.48	0.49
2:D:116:ILE:O	2:D:295:ARG:NH1	2.44	0.49
3:G:51:LEU:HD23	3:G:52:TYR:N	2.28	0.49
1:A:206:ILE:HD11	1:A:247:PRO:HG3	1.95	0.49
2:E:331:ALA:O	2:E:332:THR:OG1	2.29	0.49
7:K:52:LEU:HD22	7:R:29:PHE:HE1	1.78	0.49
7:M:25:ILE:HD12	7:M:54:PHE:HD1	1.77	0.49
8:S:138:LEU:HD22	8:S:166:ILE:HD11	1.94	0.49
2:E:26:ASP:OD1	2:E:27:GLU:N	2.43	0.49
2:F:452:LEU:HD22	2:F:470:ALA:CB	2.42	0.49
7:P:59:ALA:HB2	10:a:159:ARG:NH1	2.28	0.49
7:R:18:VAL:O	7:R:21:SER:OG	2.31	0.49
15:b:190:GLU:O	15:b:193:THR:OG1	2.26	0.49
7:P:8:PHE:CE2	7:Q:7:LYS:CD	2.90	0.49
1:C:410:LEU:HD11	6:J:32:ARG:HH22	1.78	0.48
2:E:138:LYS:NZ	2:E:460:VAL:O	2.44	0.48
4:H:52:VAL:HG22	4:H:53:PRO:HD2	1.95	0.48
10:a:85:LEU:HD12	22:b:302:CDL:H222	1.95	0.48
4:H:35:GLN:OE1	4:H:48:LEU:HD13	2.12	0.48
4:H:40:THR:HG21	4:H:45:PHE:CE1	2.47	0.48
2:D:162:LYS:N	21:D:600:ADP:O1B	2.46	0.48
2:D:250:ASP:OD1	2:D:250:ASP:O	2.31	0.48
2:E:154:LEU:HD21	2:E:162:LYS:HG3	1.95	0.48
3:G:205:GLN:OE1	3:G:205:GLN:HA	2.13	0.48
7:O:56:LEU:HD11	10:a:141:LEU:HD13	1.93	0.48
10:a:81:SER:O	10:a:85:LEU:HD13	2.13	0.48
12:f:56:ILE:O	12:f:56:ILE:HG22	2.14	0.48
13:g:37:LEU:O	18:e:15:TYR:OH	2.28	0.48
10:a:160:LEU:O	10:a:161:THR:C	2.54	0.48
10:a:191:ILE:O	10:a:194:THR:OG1	2.19	0.48
11:d:157:ILE:HG13	11:d:158:GLU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:161:VAL:O	15:b:164:MET:HG3	2.13	0.48
1:C:139:ARG:NH2	1:C:307:GLU:O	2.39	0.48
1:C:258:ARG:NH1	1:C:308:ARG:O	2.47	0.48
4:H:35:GLN:OE1	4:H:35:GLN:HA	2.12	0.48
10:a:47:GLN:NE2	10:a:47:GLN:HA	2.29	0.48
13:g:32:TYR:O	13:g:36:GLU:OE1	2.31	0.48
15:b:125:PHE:O	15:b:129:ARG:HG2	2.14	0.48
2:F:255:ILE:HG21	2:F:258:ILE:HD13	1.95	0.48
7:L:21:SER:OG	7:M:60:MET:HE1	2.13	0.48
7:O:12:GLY:O	7:O:15:THR:HG22	2.14	0.48
2:D:393:MET:HE1	2:D:404:VAL:HG11	1.96	0.48
7:N:42:LEU:O	7:N:44:GLN:N	2.47	0.48
7:P:42:LEU:O	7:P:43:M3L:C	2.62	0.48
10:a:166:ALA:O	10:a:167:GLY:C	2.55	0.48
11:d:158:GLU:N	11:d:158:GLU:OE1	2.38	0.48
16:h:57:THR:OG1	16:h:58:PHE:N	2.47	0.48
1:A:334:VAL:HG12	1:A:334:VAL:O	2.14	0.48
2:D:400:ASP:O	2:D:403:THR:N	2.46	0.48
2:D:452:LEU:HD22	2:D:470:ALA:HB1	1.96	0.48
4:H:26:VAL:HG13	4:H:26:VAL:O	2.13	0.48
16:h:35:TYR:O	16:h:39:LEU:HG	2.14	0.48
10:a:165:THR:HG23	10:a:166:ALA:N	2.29	0.48
11:d:143:LYS:C	11:d:144:LEU:HD12	2.38	0.48
1:A:28:THR:CG2	1:A:87:ILE:HG23	2.43	0.47
1:C:367:VAL:HG12	1:C:368:GLY:N	2.30	0.47
2:F:258:ILE:HG13	2:F:258:ILE:O	2.15	0.47
11:d:133:GLU:O	11:d:137:GLU:OE1	2.31	0.47
16:h:44:PHE:O	16:h:48:GLN:OE1	2.31	0.47
1:A:38:ILE:HD13	1:A:74:VAL:HG12	1.96	0.47
1:B:203:TYR:OH	1:B:269:ASP:OD1	2.25	0.47
1:C:180:ILE:CG1	1:C:216:LEU:HD11	2.44	0.47
2:E:464:GLU:OE1	2:E:464:GLU:N	2.38	0.47
7:N:21:SER:C	7:O:60:MET:HE3	2.39	0.47
7:R:60:MET:HE3	7:Q:22:GLY:CA	2.43	0.47
15:b:164:MET:CE	16:h:42:GLU:OE2	2.62	0.47
7:Q:16:VAL:O	7:Q:16:VAL:HG12	2.13	0.47
1:A:147:GLN:O	1:A:185:ASN:ND2	2.47	0.47
1:B:180:ILE:HD11	1:B:216:LEU:HD11	1.96	0.47
2:D:354:THR:HG22	2:D:355:SER:N	2.30	0.47
2:F:197:TYR:CE2	2:F:201:ILE:HD11	2.49	0.47
10:a:40:ASN:O	10:a:44:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:THR:HG23	1:C:93:ALA:H	1.80	0.47
7:R:16:VAL:O	7:R:16:VAL:CG1	2.62	0.47
8:S:55:LEU:HD13	8:S:95:LEU:CD1	2.45	0.47
10:a:160:LEU:HD11	10:a:214:PHE:CD1	2.48	0.47
11:d:111:ILE:HD11	15:b:111:GLU:CB	2.44	0.47
15:b:174:ILE:O	15:b:175:ASN:C	2.56	0.47
18:e:34:PRO:O	18:e:37:GLU:HG2	2.14	0.47
1:B:496:LYS:O	1:B:497:LEU:C	2.57	0.47
14:j:6:ILE:O	14:j:10:TRP:N	2.46	0.47
1:A:52:MET:CG	1:A:95:VAL:HG22	2.44	0.47
1:A:157:VAL:HG13	1:A:157:VAL:O	2.13	0.47
1:B:298:VAL:O	1:B:298:VAL:HG22	2.15	0.47
2:D:296:ILE:O	2:D:296:ILE:HG22	2.13	0.47
2:E:305:THR:HG22	2:E:306:SER:N	2.30	0.47
2:F:205:VAL:HG12	2:F:205:VAL:O	2.15	0.47
7:K:13:ALA:O	7:K:14:ALA:C	2.58	0.47
9:8:27:LYS:NZ	10:a:28:SER:C	2.73	0.47
11:d:18:ILE:CG2	11:d:19:ILE:N	2.77	0.47
12:f:11:LEU:C	12:f:11:LEU:HD23	2.40	0.47
2:F:416:GLN:NE2	2:F:430:LYS:O	2.47	0.47
8:S:131:LEU:HD22	8:S:152:VAL:HG21	1.97	0.47
17:k:19:ASN:OD1	17:k:22:THR:N	2.42	0.47
2:E:162:LYS:N	21:E:600:ADP:O3B	2.42	0.47
5:I:43:LYS:HE3	5:I:43:LYS:HA	1.96	0.47
7:P:33:ILE:HD11	7:Q:49:TYR:CB	2.44	0.47
7:P:60:MET:HG3	7:O:18:VAL:CG1	2.45	0.47
7:O:25:ILE:HD12	7:O:54:PHE:CD1	2.50	0.47
9:8:3:GLN:C	9:8:4:LEU:HD22	2.39	0.47
10:a:13:VAL:O	10:a:13:VAL:HG23	2.15	0.47
10:a:155:ALA:O	10:a:158:VAL:HG12	2.14	0.47
10:a:222:LEU:O	10:a:226:THR:N	2.48	0.47
15:b:63:THR:O	15:b:67:LEU:HD23	2.15	0.47
7:Q:66:MET:HG3	7:Q:67:VAL:N	2.30	0.47
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.97	0.47
2:E:232:VAL:O	2:E:232:VAL:HG22	2.14	0.47
3:G:104:LYS:HB3	3:G:125:LEU:HG	1.97	0.47
18:e:34:PRO:O	18:e:37:GLU:CG	2.62	0.47
1:A:446:TYR:OH	1:A:494:ASP:OD1	2.15	0.46
2:D:108:ILE:HG22	2:D:110:THR:HG23	1.96	0.46
2:F:97:VAL:HG13	2:F:98:ILE:HG23	1.97	0.46
3:G:57:ILE:HD12	3:G:57:ILE:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:15:VAL:O	6:J:15:VAL:HG12	2.15	0.46
1:B:75:VAL:HG11	1:B:82:ILE:CD1	2.44	0.46
1:B:390:MET:CE	1:B:428:LEU:HD21	2.39	0.46
2:E:42:GLU:OE1	2:E:42:GLU:N	2.48	0.46
7:O:21:SER:HB2	7:O:61:GLY:HA3	1.97	0.46
9:8:1:MET:HA	9:8:1:MET:HE2	1.97	0.46
11:d:107:SER:O	11:d:111:ILE:HG12	2.15	0.46
15:b:150:GLU:HG3	15:b:151:VAL:N	2.30	0.46
18:e:35:ARG:HA	18:e:38:GLU:CD	2.41	0.46
7:K:24:GLY:O	7:K:28:VAL:HG23	2.16	0.46
9:8:32:ASN:OD1	9:8:34:TYR:CD1	2.68	0.46
1:A:34:ILE:HG22	2:D:52:HIS:HB2	1.97	0.46
2:F:388:ILE:HD11	2:F:404:VAL:HG21	1.97	0.46
4:H:85:ASN:OD1	4:H:91:GLN:NE2	2.40	0.46
16:h:39:LEU:O	16:h:43:LEU:HG	2.16	0.46
18:e:35:ARG:HA	18:e:38:GLU:OE2	2.15	0.46
1:A:156:LEU:CD1	1:A:367:VAL:HG11	2.46	0.46
7:O:1:ASP:OD1	7:O:3:ASP:N	2.48	0.46
9:8:27:LYS:NZ	10:a:28:SER:OG	2.28	0.46
10:a:115:THR:HG22	10:a:119:ASN:ND2	2.31	0.46
11:d:130:MET:O	11:d:131:THR:HG23	2.15	0.46
15:b:122:HIS:ND1	15:b:126:ASP:OD2	2.49	0.46
7:Q:63:PHE:O	7:Q:66:MET:CG	2.59	0.46
7:R:6:ALA:HB1	7:Q:9:ILE:HG13	1.97	0.46
1:C:274:GLN:OE1	1:C:301:LEU:HD21	2.16	0.46
2:E:195:ASP:O	2:E:199:GLU:HG2	2.16	0.46
2:E:317:LEU:HD22	2:E:326:PHE:HE2	1.80	0.46
2:F:362:ILE:HG22	2:F:362:ILE:O	2.16	0.46
6:J:37:ARG:HA	6:J:37:ARG:NE	2.30	0.46
7:M:16:VAL:HG23	7:N:16:VAL:HG13	1.97	0.46
7:R:60:MET:CE	7:Q:25:ILE:HD12	2.46	0.46
18:e:37:GLU:HA	18:e:40:ARG:NH2	2.31	0.46
7:K:59:ALA:O	7:K:62:LEU:HG	2.15	0.46
7:N:15:THR:HG21	7:O:14:ALA:HB1	1.97	0.46
15:b:81:PHE:CE1	15:b:85:LEU:HD11	2.51	0.46
16:h:44:PHE:C	16:h:48:GLN:OE1	2.59	0.46
8:S:178:LYS:O	8:S:182:LEU:HD13	2.16	0.46
1:A:74:VAL:O	1:A:74:VAL:HG23	2.15	0.45
1:B:194:ASP:OD1	1:B:194:ASP:N	2.49	0.45
1:C:397:TYR:O	1:C:401:ALA:N	2.48	0.45
2:D:10:THR:HG23	2:D:10:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:358:MET:HE2	2:E:358:MET:HA	1.97	0.45
2:E:412:ARG:O	2:E:415:SER:OG	2.32	0.45
2:F:124:VAL:HG22	2:F:124:VAL:O	2.16	0.45
8:S:131:LEU:CD2	8:S:152:VAL:HG21	2.46	0.45
8:S:159:MET:HB3	15:b:185:ILE:HD13	1.98	0.45
10:a:73:MET:O	10:a:77:LEU:HD23	2.15	0.45
10:a:87:LEU:HD11	10:a:203:GLU:HB3	1.98	0.45
10:a:175:GLY:O	10:a:178:THR:HG22	2.16	0.45
11:d:85:TYR:O	11:d:87:ALA:N	2.49	0.45
11:d:93:GLU:O	11:d:97:VAL:HG23	2.16	0.45
12:f:61:MET:HE1	15:b:16:LEU:O	2.16	0.45
1:A:377:ALA:O	1:A:378:ALA:HB3	2.16	0.45
1:A:388:GLY:O	1:A:392:LEU:HD23	2.15	0.45
1:B:390:MET:HE1	1:B:428:LEU:CD2	2.38	0.45
1:C:180:ILE:HG22	1:C:184:ILE:HD12	1.99	0.45
3:G:72:SER:OG	3:G:85:VAL:HG21	2.16	0.45
7:O:32:LEU:HD23	7:O:32:LEU:C	2.42	0.45
10:a:64:LYS:O	10:a:67:THR:OG1	2.27	0.45
2:F:192:GLU:OE2	24:F:702:HOH:O	2.20	0.45
7:K:52:LEU:HD22	7:R:29:PHE:CE1	2.51	0.45
1:C:460:LYS:O	1:C:461:ILE:C	2.58	0.45
8:S:87:ASN:O	8:S:90:ALA:N	2.50	0.45
10:a:116:GLY:O	10:a:120:LYS:O	2.34	0.45
10:a:155:ALA:O	10:a:156:LEU:C	2.59	0.45
11:d:18:ILE:HD11	15:b:121:ARG:HA	1.98	0.45
13:g:46:PRO:O	13:g:49:ILE:HG22	2.16	0.45
1:C:36:ASP:OD2	2:F:274:ARG:NH1	2.47	0.45
7:R:63:PHE:O	7:R:66:MET:HG3	2.15	0.45
10:a:106:ILE:N	10:a:107:PRO:CD	2.80	0.45
2:D:14:VAL:HG22	2:D:22:ASP:O	2.17	0.45
2:D:298:THR:HG23	2:D:303:SER:HA	1.99	0.45
2:E:337:ARG:HH11	2:E:337:ARG:HG2	1.81	0.45
7:L:5:ALA:HB1	7:M:6:ALA:HB2	1.97	0.45
10:a:216:LEU:O	10:a:216:LEU:HD12	2.17	0.45
15:b:58:PHE:HA	15:b:61:ILE:HG22	1.98	0.45
1:A:271:LEU:HD12	1:A:325:PRO:CB	2.46	0.45
1:B:175:LYS:HD2	1:B:326:VAL:HG13	1.99	0.45
1:B:468:PHE:CE2	1:B:472:VAL:HG11	2.52	0.45
7:O:62:LEU:C	7:O:62:LEU:HD12	2.42	0.45
11:d:88:GLN:O	11:d:91:ALA:HB3	2.16	0.45
16:h:21:LYS:CE	16:h:29:VAL:HG12	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:40:ASP:O	16:h:44:PHE:CD1	2.69	0.45
7:Q:7:LYS:NZ	7:Q:75:MET:SD	2.84	0.45
1:A:323:ALA:O	1:A:324:LEU:HD23	2.16	0.45
3:G:101:LYS:O	3:G:103:VAL:HG23	2.16	0.45
7:L:35:GLY:O	7:L:36:TYR:C	2.59	0.45
13:g:71:GLU:OE1	13:g:74:LEU:HD23	2.16	0.45
1:A:179:ALA:HB1	1:A:267:ILE:HD13	1.97	0.45
1:C:390:MET:HE1	1:C:428:LEU:HD21	1.98	0.45
1:C:474:SER:OG	1:C:475:GLN:N	2.50	0.45
7:L:5:ALA:HB1	7:M:6:ALA:CB	2.47	0.45
7:P:38:ARG:NH2	7:Q:38:ARG:NH2	2.65	0.45
7:R:7:LYS:HD2	7:R:71:ILE:O	2.17	0.45
10:a:40:ASN:ND2	12:f:49:VAL:HG12	2.32	0.45
10:a:175:GLY:O	10:a:176:GLY:C	2.59	0.45
12:f:14:VAL:HG21	12:f:22:TRP:CD1	2.52	0.45
1:A:463:LYS:O	1:A:464:PHE:C	2.59	0.45
2:D:250:ASP:OD1	2:D:250:ASP:C	2.60	0.45
2:E:35:ALA:O	2:E:78:SER:OG	2.32	0.45
2:E:256:ASP:HA	2:E:257:ASN:HA	1.80	0.45
7:P:33:ILE:HG21	7:Q:32:LEU:HA	1.99	0.45
1:A:464:PHE:O	1:A:465:GLU:C	2.60	0.44
2:F:105:ARG:NH1	2:F:208:LEU:HD13	2.32	0.44
2:F:237:LEU:CD1	2:F:296:ILE:HG13	2.47	0.44
4:H:107:ALA:O	4:H:111:ASN:ND2	2.43	0.44
7:K:16:VAL:HG12	7:R:16:VAL:HG22	1.95	0.44
10:a:106:ILE:HG12	14:j:31:MET:HE2	1.99	0.44
11:d:39:SER:O	11:d:43:THR:HG23	2.17	0.44
3:G:111:LYS:O	3:G:115:ILE:HG22	2.17	0.44
15:b:33:GLY:N	15:b:34:PRO:HD2	2.33	0.44
15:b:170:GLN:O	15:b:174:ILE:HG12	2.17	0.44
18:e:53:GLN:HA	18:e:56:ILE:HG12	2.00	0.44
1:A:66:LEU:CD2	1:A:71:VAL:HG23	2.44	0.44
1:B:2:LYS:C	1:B:3:THR:HG1	2.21	0.44
7:K:60:MET:CE	7:R:22:GLY:HA2	2.47	0.44
8:S:147:VAL:HG12	8:S:148:LEU:N	2.32	0.44
11:d:31:LYS:O	11:d:35:GLU:OE1	2.35	0.44
15:b:144:LEU:O	15:b:147:VAL:HG12	2.17	0.44
18:e:18:LEU:HD23	18:e:18:LEU:C	2.41	0.44
1:A:298:VAL:HG21	1:A:338:ILE:HD11	1.98	0.44
1:C:390:MET:SD	1:C:445:ILE:HD12	2.58	0.44
1:C:504:PHE:O	1:C:508:PHE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:a:40:ASN:HD22	12:f:49:VAL:HG12	1.83	0.44
10:a:94:PRO:HB2	10:a:100:MET:SD	2.57	0.44
10:a:130:PRO:CG	10:a:141:LEU:HD21	2.47	0.44
15:b:109:ASP:OD1	15:b:109:ASP:C	2.60	0.44
16:h:16:ARG:NH1	16:h:17:GLU:HG3	2.33	0.44
1:A:8:VAL:HG12	1:A:12:LEU:CD1	2.48	0.44
2:E:316:ASP:OD1	3:G:251:ASN:CG	2.60	0.44
7:M:29:PHE:O	7:M:33:ILE:HG12	2.18	0.44
16:h:12:VAL:O	16:h:16:ARG:HD2	2.17	0.44
1:A:9:SER:HB3	16:h:18:TYR:CE1	2.53	0.44
1:B:140:ILE:HG23	1:B:313:ASN:HB3	2.00	0.44
2:E:9:THR:HG23	2:E:27:GLU:CG	2.47	0.44
2:E:152:ILE:HG22	2:E:153:GLY:N	2.32	0.44
7:L:9:ILE:HD12	7:M:9:ILE:HG22	1.99	0.44
7:L:25:ILE:HA	7:L:28:VAL:HG12	1.98	0.44
7:O:56:LEU:N	7:O:56:LEU:HD12	2.33	0.44
15:b:168:LYS:HE3	16:h:39:LEU:HD21	1.98	0.44
19:B:600:ATP:O1G	2:E:356:ARG:NH1	2.46	0.44
1:C:464:PHE:O	1:C:465:GLU:C	2.60	0.44
2:E:55:GLU:OE1	8:S:17:ARG:NE	2.51	0.44
2:F:298:THR:HG23	2:F:303:SER:CB	2.48	0.44
7:M:70:LEU:C	7:M:70:LEU:HD23	2.42	0.44
15:b:76:ALA:O	15:b:77:SER:C	2.59	0.44
1:A:139:ARG:NH2	1:A:307:GLU:O	2.43	0.44
1:A:205:ALA:HB1	1:A:208:GLN:NE2	2.33	0.44
1:C:449:VAL:O	1:C:449:VAL:HG22	2.18	0.44
3:G:48:SER:HB3	3:G:211:ASN:ND2	2.32	0.44
4:H:37:ASP:HB2	4:H:64:VAL:HG22	2.00	0.44
4:H:59:ARG:O	4:H:60:PRO:C	2.61	0.44
4:H:141:LEU:C	4:H:141:LEU:HD23	2.43	0.44
7:K:1:ASP:OD1	7:K:2:ILE:N	2.51	0.44
7:N:63:PHE:O	7:N:66:MET:HG3	2.17	0.44
11:d:40:ARG:HH12	11:d:44:LEU:HD23	1.83	0.44
1:B:389:THR:CG2	1:B:449:VAL:HG21	2.43	0.44
19:C:600:ATP:O1G	2:F:356:ARG:NH2	2.51	0.44
2:E:457:PHE:O	2:E:460:VAL:HG22	2.18	0.44
1:C:327:ILE:HD11	1:C:342:VAL:HG21	2.00	0.43
1:C:413:ALA:HB3	6:J:39:LYS:HE3	1.99	0.43
2:F:57:THR:HG22	2:F:58:VAL:N	2.32	0.43
9:8:31:HIS:HB2	11:d:152:TRP:HH2	1.82	0.43
11:d:33:TRP:O	11:d:37:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:SER:OG	1:A:409:ASP:N	2.52	0.43
1:B:71:VAL:HG12	1:B:72:GLY:N	2.33	0.43
1:C:463:LYS:O	1:C:464:PHE:C	2.61	0.43
2:D:463:ILE:O	2:D:466:ALA:HB3	2.17	0.43
3:G:81:ILE:HG22	3:G:171:TYR:CZ	2.53	0.43
11:d:43:THR:OG1	11:d:44:LEU:N	2.51	0.43
11:d:122:ARG:CZ	11:d:122:ARG:HA	2.48	0.43
11:d:156:PRO:HB2	11:d:159:THR:HG23	1.99	0.43
1:B:439:GLU:O	1:B:442:VAL:HG22	2.18	0.43
2:F:455:GLN:H	2:F:455:GLN:CD	2.26	0.43
7:N:15:THR:O	7:N:18:VAL:HG22	2.17	0.43
10:a:53:VAL:HG11	10:a:73:MET:HE1	1.99	0.43
4:H:108:ALA:HB1	4:H:141:LEU:HD22	2.00	0.43
7:N:59:ALA:C	7:N:60:MET:HE2	2.44	0.43
15:b:42:ILE:HD12	15:b:42:ILE:H	1.82	0.43
1:B:348:GLY:C	1:B:349:GLN:HG3	2.43	0.43
7:L:1:ASP:O	7:L:4:THR:OG1	2.37	0.43
7:N:58:GLU:OE2	7:O:60:MET:SD	2.76	0.43
7:R:60:MET:HE1	7:Q:21:SER:OG	2.15	0.43
11:d:51:ILE:HD11	15:b:151:VAL:CG1	2.48	0.43
11:d:91:ALA:O	11:d:92:GLU:C	2.61	0.43
12:f:52:LYS:HZ3	15:b:6:PRO:C	2.24	0.43
15:b:157:TYR:HB3	16:h:55:MET:HE2	2.00	0.43
17:k:38:ALA:HA	17:k:41:VAL:HG12	2.00	0.43
1:B:374:VAL:O	1:B:374:VAL:HG12	2.18	0.43
1:C:361:ILE:H	1:C:361:ILE:HD12	1.83	0.43
2:D:397:SER:OG	2:D:398:GLU:N	2.51	0.43
7:R:60:MET:HE2	7:Q:25:ILE:HD12	2.00	0.43
7:O:39:ASN:N	7:O:40:PRO:HD3	2.34	0.43
10:a:94:PRO:O	10:a:100:MET:SD	2.76	0.43
15:b:136:LEU:O	15:b:139:THR:OG1	2.34	0.43
15:b:195:ALA:O	15:b:198:ILE:HG22	2.19	0.43
16:h:19:ARG:O	16:h:23:GLN:NE2	2.52	0.43
1:A:47:VAL:HG13	1:A:47:VAL:O	2.19	0.43
2:F:119:GLU:N	2:F:119:GLU:OE2	2.52	0.43
15:b:173:MET:HE1	16:h:21:LYS:HZ1	1.82	0.43
1:A:342:VAL:HG12	1:A:342:VAL:O	2.19	0.43
1:C:180:ILE:HD11	1:C:216:LEU:CD1	2.45	0.43
1:C:460:LYS:O	1:C:463:LYS:HG2	2.19	0.43
3:G:74:ASP:OD1	3:G:74:ASP:N	2.45	0.43
8:S:5:VAL:HG23	8:S:5:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:VAL:HG11	8:S:173:MET:HG2	2.01	0.43
1:A:96:ASP:OD1	1:A:96:ASP:N	2.51	0.43
2:D:385:GLN:HG2	6:J:26:GLU:OE2	2.19	0.43
15:b:123:TYR:O	15:b:127:VAL:HG23	2.18	0.43
2:E:154:LEU:HD11	2:E:335:LEU:HD11	2.01	0.43
2:E:339:ILE:HG22	2:E:339:ILE:O	2.19	0.43
2:F:218:VAL:HG12	2:F:232:VAL:HG23	2.01	0.43
7:K:54:PHE:CZ	7:L:56:LEU:HD21	2.54	0.43
9:8:31:HIS:HB3	10:a:47:GLN:HE22	1.83	0.43
15:b:92:GLN:O	15:b:95:GLU:HG3	2.19	0.43
1:A:32:LEU:HD11	1:A:42:HIS:HB2	2.01	0.42
1:C:139:ARG:HB2	2:D:194:ASN:ND2	2.34	0.42
1:C:461:ILE:O	1:C:462:THR:C	2.62	0.42
2:E:224:GLU:CG	2:E:225:PRO:HD2	2.49	0.42
7:N:22:GLY:N	7:O:60:MET:HE3	2.34	0.42
7:P:55:ALA:HB2	10:a:213:VAL:HG21	1.99	0.42
8:S:172:ASP:C	8:S:172:ASP:OD2	2.62	0.42
10:a:195:ILE:HD12	10:a:195:ILE:H	1.84	0.42
11:d:40:ARG:NH2	15:b:138:VAL:HG13	2.34	0.42
18:e:9:LEU:C	18:e:9:LEU:HD23	2.44	0.42
1:A:353:GLU:OE1	1:A:366:ASN:ND2	2.52	0.42
1:A:462:THR:HG23	1:A:463:LYS:N	2.34	0.42
1:C:163:GLN:O	1:C:322:THR:HG23	2.20	0.42
2:E:186:VAL:HG22	2:E:232:VAL:HG13	2.01	0.42
7:M:56:LEU:C	7:M:56:LEU:HD23	2.45	0.42
7:N:16:VAL:HG23	7:O:16:VAL:HG13	2.00	0.42
7:N:42:LEU:C	7:N:44:GLN:H	2.27	0.42
8:S:60:VAL:O	8:S:61:LYS:C	2.62	0.42
1:C:41:VAL:HG11	1:C:44:LEU:HD12	2.02	0.42
2:D:103:ASP:OD1	2:D:103:ASP:N	2.45	0.42
2:D:391:LEU:CG	3:G:23:MET:HE1	2.47	0.42
2:E:402:LEU:HD11	2:E:450:ASP:OD2	2.20	0.42
7:P:42:LEU:HD13	7:O:36:TYR:CE2	2.54	0.42
10:a:137:LEU:C	10:a:137:LEU:HD12	2.44	0.42
11:d:144:LEU:O	11:d:145:ASP:OD1	2.36	0.42
1:A:163:GLN:NE2	1:A:165:GLU:OE1	2.52	0.42
1:B:20:ASP:N	1:B:20:ASP:OD1	2.52	0.42
2:D:260:ARG:NH1	2:D:263:GLN:OE1	2.52	0.42
2:E:244:ARG:NH1	2:E:304:ILE:HD12	2.34	0.42
2:F:285:LEU:C	2:F:285:LEU:HD23	2.44	0.42
4:H:22:SER:OG	4:H:23:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:33:PHE:HZ	10:a:50:LEU:HB3	1.84	0.42
10:a:199:LEU:O	10:a:203:GLU:HG2	2.20	0.42
10:a:210:GLN:HA	10:a:213:VAL:HG12	2.02	0.42
14:j:6:ILE:HG23	14:j:10:TRP:HB2	2.01	0.42
15:b:197:CYS:O	15:b:201:LEU:HD23	2.18	0.42
1:A:71:VAL:O	1:A:71:VAL:HG13	2.20	0.42
1:A:271:LEU:HD12	1:A:325:PRO:HB2	2.00	0.42
1:C:309:ALA:HB1	1:C:321:LEU:O	2.19	0.42
3:G:70:GLY:HA3	3:G:89:MET:SD	2.59	0.42
7:P:49:TYR:HB3	7:O:33:ILE:HD11	2.00	0.42
8:S:98:THR:N	8:S:99:PRO:HD2	2.35	0.42
10:a:43:VAL:O	10:a:47:GLN:HG2	2.19	0.42
12:f:50:ASN:OD1	15:b:5:LEU:HD22	2.19	0.42
15:b:157:TYR:CG	16:h:55:MET:HE2	2.55	0.42
1:C:489:ILE:O	1:C:489:ILE:HG22	2.20	0.42
2:E:173:VAL:HG21	2:E:252:LEU:CD2	2.48	0.42
2:F:393:MET:O	2:F:401:LYS:NZ	2.37	0.42
3:G:12:SER:OG	6:J:18:ALA:HB2	2.20	0.42
7:K:14:ALA:HB1	7:R:15:THR:HG21	2.02	0.42
7:P:16:VAL:HG13	7:O:16:VAL:HG23	2.01	0.42
15:b:39:THR:HG23	15:b:40:GLY:N	2.35	0.42
3:G:112:ILE:HA	3:G:115:ILE:HG22	2.01	0.42
7:N:59:ALA:HB3	7:N:60:MET:HE2	2.01	0.42
7:R:9:ILE:CG2	7:Q:9:ILE:HG12	2.50	0.42
11:d:10:ILE:CD1	15:b:127:VAL:HG22	2.49	0.42
13:g:75:ASN:O	13:g:78:VAL:HG12	2.19	0.42
7:Q:62:LEU:CD2	7:Q:65:LEU:HD23	2.48	0.42
1:A:386:VAL:HG11	1:A:445:ILE:HB	2.02	0.42
1:B:78:ASN:OD1	1:B:80:LYS:HB3	2.20	0.42
1:B:505:LEU:O	1:B:506:ALA:C	2.63	0.42
1:C:269:ASP:HA	1:C:270:ASP:HA	1.84	0.42
2:E:262:THR:HG22	2:E:289:MET:HE1	2.01	0.42
2:F:45:LEU:HD12	2:F:64:ASP:HB3	2.02	0.42
2:F:279:VAL:O	2:F:279:VAL:CG1	2.67	0.42
3:G:126:VAL:HG12	3:G:127:THR:N	2.35	0.42
8:S:116:VAL:HG21	8:S:142:LEU:HD22	2.01	0.42
10:a:170:LEU:HD13	7:Q:66:MET:HB3	2.01	0.42
10:a:174:ILE:O	10:a:175:GLY:C	2.62	0.42
11:d:144:LEU:O	11:d:145:ASP:C	2.61	0.42
15:b:146:ARG:HE	16:h:63:PHE:HE1	1.67	0.42
2:D:374:VAL:O	2:D:377:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:164:ARG:HD2	3:G:174:GLU:HG3	2.02	0.42
5:I:45:VAL:HG23	5:I:45:VAL:O	2.20	0.42
8:S:66:VAL:HG13	8:S:87:ASN:OD1	2.19	0.42
9:8:12:MET:SD	10:a:20:VAL:HG21	2.59	0.42
10:a:100:MET:HE2	10:a:104:MET:HE3	2.01	0.42
11:d:151:TYR:O	11:d:154:HIS:ND1	2.53	0.42
1:A:159:ILE:HD11	1:A:350:ILE:HD11	2.02	0.42
1:A:248:TYR:OH	1:A:301:LEU:HD12	2.20	0.42
7:R:4:THR:O	7:R:7:LYS:HB3	2.20	0.42
18:e:45:GLU:O	18:e:48:LYS:HG2	2.19	0.42
2:E:81:PRO:O	2:E:82:ILE:C	2.63	0.41
2:E:139:VAL:HG13	2:E:140:VAL:N	2.35	0.41
2:F:298:THR:O	2:F:298:THR:HG22	2.20	0.41
3:G:196:ILE:O	3:G:196:ILE:HG13	2.20	0.41
7:P:73:PHE:O	7:P:74:ALA:HB2	2.20	0.41
7:R:14:ALA:CB	7:Q:15:THR:CG2	2.98	0.41
10:a:159:ARG:O	10:a:160:LEU:C	2.63	0.41
11:d:44:LEU:C	11:d:44:LEU:HD12	2.45	0.41
15:b:71:VAL:HG13	15:b:72:LYS:N	2.34	0.41
15:b:173:MET:SD	16:h:21:LYS:NZ	2.90	0.41
7:Q:65:LEU:HD11	7:Q:69:PHE:CE1	2.55	0.41
1:B:218:LYS:HG3	2:E:128:VAL:HG21	2.02	0.41
1:B:498:LYS:O	1:B:501:VAL:HG12	2.20	0.41
1:C:129:VAL:HG23	1:C:130:GLY:N	2.35	0.41
1:C:230:ILE:HG22	1:C:231:VAL:N	2.34	0.41
2:D:347:ALA:O	2:D:348:VAL:C	2.63	0.41
3:G:59:THR:HG21	3:G:157:GLU:CD	2.44	0.41
3:G:128:PHE:HB3	5:I:42:ILE:HD11	2.02	0.41
7:M:37:ALA:HB2	7:N:46:LEU:HD21	2.02	0.41
7:P:29:PHE:O	7:P:33:ILE:HG12	2.20	0.41
7:R:63:PHE:HA	7:R:66:MET:HG3	2.02	0.41
10:a:58:MET:HE3	10:a:58:MET:HA	2.02	0.41
11:d:40:ARG:NH2	11:d:41:LEU:HA	2.35	0.41
1:A:382:ALA:N	1:A:487:GLY:O	2.51	0.41
1:B:464:PHE:O	1:B:465:GLU:C	2.63	0.41
1:B:489:ILE:O	1:B:489:ILE:HG22	2.18	0.41
2:E:141:ASP:O	2:E:141:ASP:OD2	2.38	0.41
2:E:182:VAL:HG12	2:E:183:PHE:H	1.85	0.41
2:F:103:ASP:OD1	2:F:103:ASP:N	2.44	0.41
7:N:66:MET:SD	7:N:67:VAL:N	2.93	0.41
7:O:25:ILE:HD12	7:O:54:PHE:HD1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASP:O	1:B:173:THR:OG1	2.38	0.41
2:F:347:ALA:O	2:F:348:VAL:C	2.62	0.41
11:d:5:LEU:HD12	11:d:5:LEU:O	2.21	0.41
1:B:434:SER:O	1:B:434:SER:OG	2.30	0.41
1:C:105:GLY:HA2	1:C:226:MET:O	2.21	0.41
1:C:403:PHE:CZ	6:J:32:ARG:CD	3.02	0.41
1:C:403:PHE:CD1	6:J:32:ARG:CZ	3.03	0.41
1:C:465:GLU:O	1:C:469:LEU:HD23	2.19	0.41
2:D:39:GLN:CG	2:D:76:LEU:HD23	2.50	0.41
2:E:53:LEU:HD11	2:E:59:ARG:HB2	2.01	0.41
2:F:94:ILE:HG22	2:F:102:ILE:HG12	2.01	0.41
2:F:298:THR:HG23	2:F:303:SER:HA	2.02	0.41
4:H:119:LEU:C	4:H:119:LEU:HD23	2.46	0.41
7:P:56:LEU:HD13	7:O:54:PHE:CD1	2.55	0.41
7:P:62:LEU:HD13	10:a:162:ALA:CB	2.38	0.41
7:R:29:PHE:O	7:R:33:ILE:HG12	2.20	0.41
10:a:86:GLY:HA3	10:a:93:THR:OG1	2.21	0.41
12:f:84:ARG:HB2	13:g:98:ILE:HD12	2.03	0.41
13:g:32:TYR:CE1	15:b:31:VAL:HG21	2.56	0.41
15:b:29:THR:CG2	15:b:33:GLY:HA3	2.48	0.41
2:D:393:MET:HG2	6:J:33:TYR:CG	2.55	0.41
2:F:252:LEU:HD23	2:F:254:PHE:CZ	2.55	0.41
3:G:89:MET:HE2	3:G:116:LEU:HD11	2.02	0.41
3:G:196:ILE:CG2	4:H:55:LEU:HB2	2.51	0.41
7:N:29:PHE:O	7:N:33:ILE:HG12	2.21	0.41
7:P:32:LEU:HA	7:O:33:ILE:HG21	2.03	0.41
7:P:47:PHE:O	7:P:49:TYR:N	2.54	0.41
11:d:109:THR:HA	11:d:112:GLN:OE1	2.19	0.41
15:b:173:MET:CE	16:h:21:LYS:NZ	2.84	0.41
16:h:42:GLU:OE2	16:h:43:LEU:HG	2.20	0.41
1:A:269:ASP:HA	1:A:270:ASP:HA	1.86	0.41
2:E:237:LEU:HD21	2:E:296:ILE:CG1	2.51	0.41
2:F:97:VAL:HG13	2:F:98:ILE:N	2.36	0.41
2:F:296:ILE:HG21	2:F:306:SER:HB2	2.02	0.41
7:L:39:ASN:ND2	7:L:42:LEU:HD12	2.36	0.41
8:S:56:LEU:HD12	8:S:56:LEU:O	2.21	0.41
8:S:173:MET:HE1	15:b:200:ASP:CB	2.50	0.41
7:O:60:MET:HG2	7:O:60:MET:O	2.21	0.41
10:a:135:THR:O	10:a:137:LEU:N	2.53	0.41
10:a:164:ILE:O	10:a:165:THR:C	2.62	0.41
11:d:44:LEU:HD13	15:b:141:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLU:HB3	1:A:68:PRO:HD2	2.01	0.41
1:B:496:LYS:O	1:B:499:GLU:HG3	2.20	0.41
1:C:156:LEU:HD13	1:C:367:VAL:HG21	2.02	0.41
1:C:397:TYR:CG	1:C:421:GLY:HA3	2.56	0.41
1:C:468:PHE:O	1:C:469:LEU:C	2.64	0.41
2:F:310:ILE:HG12	2:F:325:THR:HG21	2.02	0.41
3:G:113:ARG:HB2	3:G:127:THR:HG21	2.03	0.41
7:P:8:PHE:HD2	7:Q:7:LYS:HG2	1.84	0.41
8:S:186:MET:HE1	15:b:174:ILE:HD12	2.02	0.41
10:a:213:VAL:O	10:a:217:LEU:HD23	2.21	0.41
11:d:51:ILE:HD11	15:b:151:VAL:HG11	2.01	0.41
13:g:84:MET:CE	15:b:40:GLY:HA3	2.48	0.41
1:A:176:THR:O	1:A:180:ILE:HG12	2.21	0.41
1:A:496:LYS:O	1:A:500:ILE:HG12	2.21	0.41
1:C:414:THR:O	1:C:418:LEU:HD23	2.21	0.41
3:G:140:ASP:OD1	5:I:42:ILE:N	2.50	0.41
7:L:42:LEU:C	7:L:44:GLN:H	2.26	0.41
7:L:72:LEU:HD23	7:L:73:PHE:CE2	2.56	0.41
7:N:24:GLY:O	7:N:27:THR:HG22	2.21	0.41
7:N:66:MET:SD	7:N:66:MET:C	3.04	0.41
8:S:103:SER:O	8:S:106:SER:OG	2.33	0.41
8:S:118:CYS:O	8:S:119:THR:OG1	2.31	0.41
9:8:34:TYR:HA	11:d:144:LEU:HD11	2.02	0.41
11:d:132:ILE:HG23	11:d:133:GLU:N	2.36	0.41
12:f:11:LEU:HA	12:f:14:VAL:HG23	2.02	0.41
13:g:83:TRP:CD1	13:g:83:TRP:C	2.98	0.41
14:j:14:LYS:N	14:j:15:PRO:HD2	2.36	0.41
15:b:176:TRP:CE3	16:h:21:LYS:HD3	2.56	0.41
1:B:47:VAL:O	1:B:47:VAL:HG13	2.20	0.41
1:C:390:MET:CE	1:C:428:LEU:HD21	2.51	0.41
2:D:310:ILE:HG22	2:D:311:TYR:O	2.20	0.41
2:F:419:GLN:NE2	2:F:431:LEU:HD11	2.36	0.41
6:J:36:ALA:HB1	6:J:37:ARG:NH2	2.36	0.41
7:N:59:ALA:CB	7:N:60:MET:HE2	2.51	0.41
7:N:66:MET:O	7:N:70:LEU:HD13	2.21	0.41
11:d:57:LYS:HB2	11:d:66:VAL:HG11	2.03	0.41
18:e:19:PHE:O	18:e:22:MET:HB2	2.21	0.41
18:e:50:ARG:O	18:e:54:LYS:HG2	2.21	0.41
1:A:374:VAL:HG23	1:A:375:GLY:N	2.36	0.40
1:B:38:ILE:CD1	1:B:285:LEU:HD22	2.51	0.40
1:B:105:GLY:HA2	1:B:226:MET:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ILE:HG22	1:B:184:ILE:HD12	2.03	0.40
1:B:248:TYR:OH	1:B:301:LEU:HD12	2.21	0.40
7:P:39:ASN:O	7:P:41:SER:N	2.54	0.40
11:d:40:ARG:NH1	11:d:44:LEU:HD23	2.36	0.40
13:g:94:LYS:O	13:g:95:ARG:C	2.64	0.40
1:B:361:ILE:O	1:B:361:ILE:HG22	2.20	0.40
7:L:4:THR:OG1	7:M:3:ASP:OD1	2.30	0.40
7:M:5:ALA:HB1	7:N:6:ALA:HB2	2.03	0.40
10:a:95:THR:HA	10:a:100:MET:SD	2.62	0.40
15:b:175:ASN:HA	15:b:178:GLU:OE2	2.21	0.40
1:A:79:ASP:OD1	1:A:79:ASP:N	2.46	0.40
1:B:38:ILE:HD12	1:B:285:LEU:HD22	2.01	0.40
1:C:403:PHE:CG	6:J:32:ARG:CZ	3.04	0.40
2:D:194:ASN:OD1	2:D:195:ASP:N	2.54	0.40
2:E:108:ILE:HG22	2:E:110:THR:HG23	2.02	0.40
7:M:52:LEU:C	7:M:52:LEU:HD23	2.46	0.40
8:S:162:MET:HE2	15:b:197:CYS:SG	2.62	0.40
9:8:31:HIS:HB2	11:d:152:TRP:CH2	2.55	0.40
18:e:50:ARG:CZ	18:e:53:GLN:OE1	2.69	0.40
1:B:292:GLU:O	1:B:293:ALA:HB3	2.22	0.40
2:D:391:LEU:CD2	3:G:23:MET:HE1	2.51	0.40
2:D:452:LEU:HD22	2:D:470:ALA:CB	2.50	0.40
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.52	0.40
2:F:366:GLU:HG2	2:F:367:HIS:N	2.36	0.40
3:G:193:TYR:CD1	4:H:55:LEU:HD23	2.57	0.40
7:P:44:GLN:O	7:P:45:GLN:C	2.64	0.40
7:P:64:CYS:SG	7:O:18:VAL:HB	2.62	0.40
8:S:19:ALA:HB1	8:S:108:MET:HE2	2.03	0.40
12:f:65:ALA:O	12:f:69:LEU:HD23	2.21	0.40
14:j:6:ILE:H	14:j:6:ILE:HD12	1.86	0.40
15:b:98:GLN:OE1	15:b:101:ILE:HD11	2.21	0.40
15:b:181:VAL:N	16:h:17:GLU:OE2	2.54	0.40
7:Q:62:LEU:HA	7:Q:65:LEU:HB3	2.03	0.40
1:B:270:ASP:HB2	1:B:326:VAL:O	2.22	0.40
1:C:155:SER:OG	1:C:156:LEU:N	2.54	0.40
2:E:48:GLU:OE2	2:E:231:ARG:NE	2.41	0.40
2:F:153:GLY:HA3	2:F:329:LEU:HD13	2.02	0.40
3:G:55:ALA:O	3:G:57:ILE:HD12	2.22	0.40
6:J:46:LYS:O	6:J:47:LYS:C	2.64	0.40
7:N:21:SER:OG	7:O:60:MET:CE	2.70	0.40
7:P:38:ARG:HH22	7:Q:38:ARG:NH2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:56:LEU:HD11	10:a:141:LEU:CD1	2.52	0.40
9:8:8:THR:O	9:8:9:TRP:C	2.64	0.40
9:8:26:LEU:HD11	14:j:9:VAL:HG22	2.03	0.40
10:a:122:LYS:HG2	17:k:27:MET:HE1	2.04	0.40
11:d:60:VAL:HA	15:b:162:GLN:OE1	2.21	0.40
15:b:168:LYS:HG2	15:b:169:GLU:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/510 (98%)	450 (90%)	49 (10%)	0	100	100
1	B	498/510 (98%)	453 (91%)	45 (9%)	0	100	100
1	C	479/510 (94%)	423 (88%)	56 (12%)	0	100	100
2	D	467/482 (97%)	430 (92%)	37 (8%)	0	100	100
2	E	465/482 (96%)	423 (91%)	42 (9%)	0	100	100
2	F	465/482 (96%)	420 (90%)	45 (10%)	0	100	100
3	G	270/273 (99%)	255 (94%)	15 (6%)	0	100	100
4	H	129/146 (88%)	115 (89%)	14 (11%)	0	100	100
5	I	45/50 (90%)	45 (100%)	0	0	100	100
6	J	45/66 (68%)	41 (91%)	4 (9%)	0	100	100
7	K	71/75 (95%)	66 (93%)	5 (7%)	0	100	100
7	L	71/75 (95%)	70 (99%)	1 (1%)	0	100	100
7	M	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
7	N	72/75 (96%)	67 (93%)	5 (7%)	0	100	100
7	O	72/75 (96%)	70 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	P	71/75 (95%)	67 (94%)	3 (4%)	1 (1%)	9	39
7	Q	72/75 (96%)	69 (96%)	3 (4%)	0	100	100
7	R	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
8	S	185/190 (97%)	173 (94%)	12 (6%)	0	100	100
9	8	39/66 (59%)	33 (85%)	6 (15%)	0	100	100
10	a	224/226 (99%)	195 (87%)	29 (13%)	0	100	100
11	d	153/160 (96%)	136 (89%)	17 (11%)	0	100	100
12	f	81/87 (93%)	71 (88%)	10 (12%)	0	100	100
13	g	77/102 (76%)	70 (91%)	7 (9%)	0	100	100
14	j	46/60 (77%)	44 (96%)	2 (4%)	0	100	100
15	b	207/214 (97%)	197 (95%)	10 (5%)	0	100	100
16	h	60/76 (79%)	53 (88%)	7 (12%)	0	100	100
17	k	34/57 (60%)	34 (100%)	0	0	100	100
18	e	54/70 (77%)	53 (98%)	1 (2%)	0	100	100
All	All	5095/5419 (94%)	4655 (91%)	439 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	P	44	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/412 (98%)	406 (100%)	0	100	100
1	B	407/412 (99%)	407 (100%)	0	100	100
1	C	391/412 (95%)	391 (100%)	0	100	100
2	D	379/386 (98%)	379 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	377/386 (98%)	377 (100%)	0	100	100
2	F	377/386 (98%)	377 (100%)	0	100	100
3	G	230/231 (100%)	230 (100%)	0	100	100
4	H	104/109 (95%)	104 (100%)	0	100	100
5	I	38/41 (93%)	38 (100%)	0	100	100
6	J	34/50 (68%)	34 (100%)	0	100	100
7	K	49/50 (98%)	49 (100%)	0	100	100
7	L	49/50 (98%)	49 (100%)	0	100	100
7	M	50/50 (100%)	50 (100%)	0	100	100
7	N	50/50 (100%)	50 (100%)	0	100	100
7	O	50/50 (100%)	49 (98%)	1 (2%)	48	66
7	P	49/50 (98%)	49 (100%)	0	100	100
7	Q	50/50 (100%)	50 (100%)	0	100	100
7	R	50/50 (100%)	50 (100%)	0	100	100
8	S	162/165 (98%)	162 (100%)	0	100	100
9	8	41/66 (62%)	41 (100%)	0	100	100
10	a	200/200 (100%)	200 (100%)	0	100	100
11	d	139/142 (98%)	139 (100%)	0	100	100
12	f	72/75 (96%)	72 (100%)	0	100	100
13	g	67/83 (81%)	67 (100%)	0	100	100
14	j	42/49 (86%)	42 (100%)	0	100	100
15	b	186/190 (98%)	186 (100%)	0	100	100
16	h	56/70 (80%)	56 (100%)	0	100	100
17	k	31/46 (67%)	31 (100%)	0	100	100
18	e	47/59 (80%)	47 (100%)	0	100	100
All	All	4183/4370 (96%)	4182 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	O	47	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	GLN
1	A	477	GLN
1	B	385	GLN
1	C	330	GLN
2	D	411	GLN
2	F	263	GLN
3	G	120	HIS
3	G	150	ASN
7	N	44	GLN
8	S	112	HIS
9	8	35	HIS
9	8	36	ASN
10	a	56	GLN
10	a	131	GLN
10	a	172	HIS
11	d	74	ASN
12	f	80	HIS
13	g	57	ASN
15	b	128	GLN
15	b	172	HIS
16	h	60	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	M3L	N	43	7	10,11,12	0.41	0	9,14,16	0.57	0
7	M3L	L	43	7	10,11,12	0.47	0	9,14,16	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	M3L	O	43	7	10,11,12	0.39	0	9,14,16	0.63	0
7	M3L	R	43	7	10,11,12	0.51	0	9,14,16	0.63	0
7	M3L	M	43	7	10,11,12	0.57	0	9,14,16	0.48	0
7	M3L	Q	43	7	10,11,12	0.52	0	9,14,16	0.49	0
7	M3L	K	43	7	10,11,12	0.50	0	9,14,16	0.52	0
7	M3L	P	43	7	10,11,12	0.47	0	9,14,16	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	M3L	N	43	7	-	1/9/10/12	-
7	M3L	L	43	7	-	1/9/10/12	-
7	M3L	O	43	7	-	3/9/10/12	-
7	M3L	R	43	7	-	1/9/10/12	-
7	M3L	M	43	7	-	2/9/10/12	-
7	M3L	Q	43	7	-	1/9/10/12	-
7	M3L	K	43	7	-	1/9/10/12	-
7	M3L	P	43	7	-	1/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	43	M3L	N-CA-CB-CG
7	O	43	M3L	N-CA-CB-CG
7	O	43	M3L	O-C-CA-CB
7	L	43	M3L	CG-CD-CE-NZ
7	R	43	M3L	CG-CD-CE-NZ
7	K	43	M3L	CE-CD-CG-CB
7	O	43	M3L	CE-CD-CG-CB
7	N	43	M3L	CG-CD-CE-NZ
7	P	43	M3L	CE-CD-CG-CB
7	M	43	M3L	C-CA-CB-CG
7	Q	43	M3L	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	43	M3L	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	LHG	f	103	-	48,48,48	0.63	1 (2%)	51,54,54	1.24	4 (7%)
22	CDL	f	101	-	83,83,99	1.00	7 (8%)	89,95,111	1.12	4 (4%)
23	LHG	f	102	-	38,38,48	0.71	1 (2%)	41,44,54	1.35	5 (12%)
19	ATP	A	600	20	32,33,33	1.28	5 (15%)	48,52,52	1.81	10 (20%)
22	CDL	b	301	-	77,77,99	1.02	6 (7%)	83,89,111	1.13	4 (4%)
21	ADP	F	600	20	28,29,29	1.37	5 (17%)	43,45,45	1.91	10 (23%)
22	CDL	b	302	-	82,82,99	0.99	6 (7%)	88,94,111	1.17	5 (5%)
21	ADP	E	600	-	28,29,29	1.38	5 (17%)	43,45,45	1.90	11 (25%)
21	ADP	D	600	20	28,29,29	1.38	5 (17%)	43,45,45	1.86	11 (25%)
19	ATP	C	600	20	32,33,33	1.31	5 (15%)	48,52,52	1.86	11 (22%)
19	ATP	B	600	20	32,33,33	1.28	5 (15%)	48,52,52	1.82	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	f	103	-	-	18/53/53/53	-
22	CDL	f	101	-	-	38/94/94/110	-
23	LHG	f	102	-	-	14/43/43/53	-
19	ATP	A	600	20	-	0/22/38/38	0/3/3/3
22	CDL	b	301	-	-	42/88/88/110	-
21	ADP	F	600	20	-	5/16/32/32	0/3/3/3
22	CDL	b	302	-	-	31/93/93/110	-
21	ADP	E	600	-	-	4/16/32/32	0/3/3/3
21	ADP	D	600	20	-	2/16/32/32	0/3/3/3
19	ATP	C	600	20	-	4/22/38/38	0/3/3/3
19	ATP	B	600	20	-	1/22/38/38	0/3/3/3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	E	600	ADP	C5-C4	4.38	1.46	1.39
21	D	600	ADP	C5-C4	4.19	1.46	1.39
21	F	600	ADP	C5-C4	4.13	1.46	1.39
19	C	600	ATP	C5-C4	4.11	1.46	1.39
19	A	600	ATP	C5-C4	4.10	1.46	1.39
19	B	600	ATP	C5-C4	4.09	1.46	1.39
22	b	301	CDL	OA6-CA4	-2.94	1.39	1.46
22	b	302	CDL	OA6-CA4	-2.93	1.39	1.46
19	A	600	ATP	C5-N7	-2.88	1.33	1.39
22	f	101	CDL	OA6-CA4	-2.84	1.39	1.46
22	f	101	CDL	OB6-CB4	-2.81	1.40	1.46
19	C	600	ATP	C5-N7	-2.79	1.34	1.39
21	D	600	ADP	C5-N7	-2.78	1.34	1.39
21	F	600	ADP	C5-N7	-2.76	1.34	1.39
19	B	600	ATP	C5-N7	-2.72	1.34	1.39
22	b	302	CDL	OB6-CB4	-2.71	1.40	1.46
22	f	101	CDL	OB8-CB7	2.70	1.41	1.33
22	b	301	CDL	OB6-CB4	-2.66	1.40	1.46
22	b	302	CDL	OB8-CB7	2.62	1.41	1.33
22	b	301	CDL	OB8-CB7	2.61	1.41	1.33
21	E	600	ADP	C5-N7	-2.54	1.34	1.39
21	E	600	ADP	C5-C6	2.52	1.48	1.41
23	f	102	LHG	O7-C5	-2.46	1.40	1.46
22	b	301	CDL	OB6-CB5	2.45	1.41	1.34
21	F	600	ADP	C5-C6	2.39	1.47	1.41
22	b	302	CDL	OA8-CA7	2.36	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	f	103	LHG	O7-C5	-2.36	1.41	1.46
22	b	302	CDL	OB6-CB5	2.35	1.40	1.34
21	D	600	ADP	C5-C6	2.34	1.47	1.41
22	f	101	CDL	OB6-CB5	2.32	1.40	1.34
21	E	600	ADP	C8-N7	2.31	1.36	1.31
22	b	301	CDL	OA8-CA6	-2.30	1.40	1.45
21	D	600	ADP	C4-N9	-2.30	1.32	1.37
22	f	101	CDL	OA8-CA6	-2.30	1.40	1.45
22	f	101	CDL	OA8-CA7	2.30	1.40	1.33
19	C	600	ATP	C4-N9	-2.25	1.33	1.37
19	C	600	ATP	C5-C6	2.24	1.47	1.41
19	B	600	ATP	C8-N7	2.22	1.35	1.31
21	F	600	ADP	C8-N7	2.21	1.35	1.31
21	D	600	ADP	C8-N7	2.20	1.35	1.31
19	B	600	ATP	C5-C6	2.20	1.47	1.41
22	b	301	CDL	OA8-CA7	2.19	1.39	1.33
19	B	600	ATP	C4-N9	-2.18	1.33	1.37
21	F	600	ADP	C4-N9	-2.15	1.33	1.37
22	b	302	CDL	OA8-CA6	-2.15	1.40	1.45
19	A	600	ATP	C4-N9	-2.15	1.33	1.37
19	A	600	ATP	C5-C6	2.15	1.47	1.41
19	C	600	ATP	C8-N7	2.14	1.35	1.31
19	A	600	ATP	C8-N7	2.10	1.35	1.31
22	f	101	CDL	OA6-CA5	2.09	1.40	1.34
21	E	600	ADP	C4-N9	-2.07	1.33	1.37

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	600	ATP	C5-C4-N3	-5.89	118.61	126.72
19	B	600	ATP	C5-C4-N3	-5.88	118.62	126.72
21	F	600	ADP	C5-C4-N3	-5.81	118.72	126.72
21	E	600	ADP	C5-C4-N3	-5.81	118.72	126.72
19	A	600	ATP	C5-C4-N3	-5.76	118.78	126.72
21	D	600	ADP	C5-C4-N3	-5.70	118.87	126.72
19	B	600	ATP	N3-C4-N9	4.85	135.42	127.17
19	A	600	ATP	N3-C4-N9	4.77	135.28	127.17
19	C	600	ATP	N3-C4-N9	4.76	135.27	127.17
21	E	600	ADP	N3-C4-N9	4.55	134.90	127.17
23	f	102	LHG	O4-P-O5	4.54	133.57	112.44
21	F	600	ADP	N3-C4-N9	4.48	134.78	127.17
23	f	103	LHG	O4-P-O5	4.45	133.16	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	600	ADP	N3-C4-N9	4.34	134.55	127.17
22	b	302	CDL	OA6-CA5-C11	4.20	120.56	111.48
22	b	302	CDL	OB6-CB5-C51	4.10	120.35	111.48
22	b	301	CDL	OB6-CB5-C51	3.99	120.12	111.48
22	f	101	CDL	OA6-CA5-C11	3.98	120.09	111.48
22	f	101	CDL	OB6-CB5-C51	3.92	119.97	111.48
22	b	301	CDL	OA6-CA5-C11	3.87	119.86	111.48
19	A	600	ATP	N3-C2-N1	-3.87	122.73	128.58
19	B	600	ATP	C2-N3-C4	3.84	121.22	111.83
21	E	600	ADP	C2-N3-C4	3.84	121.21	111.83
19	A	600	ATP	C2-N3-C4	3.83	121.19	111.83
21	F	600	ADP	C2-N3-C4	3.82	121.16	111.83
19	B	600	ATP	N3-C2-N1	-3.76	122.89	128.58
19	C	600	ATP	C2-N3-C4	3.75	120.98	111.83
21	D	600	ADP	C2-N3-C4	3.74	120.96	111.83
21	E	600	ADP	N3-C2-N1	-3.68	123.01	128.58
21	F	600	ADP	N3-C2-N1	-3.65	123.06	128.58
21	D	600	ADP	N3-C2-N1	-3.62	123.11	128.58
21	E	600	ADP	C4-C5-N7	-3.57	106.50	110.58
21	F	600	ADP	C4-C5-N7	-3.56	106.51	110.58
19	C	600	ATP	N3-C2-N1	-3.53	123.24	128.58
21	D	600	ADP	C4-C5-N7	-3.46	106.63	110.58
19	C	600	ATP	C4-C5-N7	-3.27	106.84	110.58
19	B	600	ATP	C4-C5-N7	-3.19	106.94	110.58
19	B	600	ATP	C4-N9-C8	3.17	109.07	105.74
19	A	600	ATP	C4-C5-N7	-3.02	107.13	110.58
19	C	600	ATP	C4-N9-C8	2.98	108.86	105.74
19	A	600	ATP	C4-N9-C8	2.87	108.75	105.74
21	E	600	ADP	C4-N9-C8	2.85	108.73	105.74
22	b	302	CDL	OA8-CA7-C31	2.85	120.52	111.83
22	b	302	CDL	OB8-CB7-C71	2.80	120.36	111.83
21	D	600	ADP	C3'-C2'-C1'	2.77	106.71	101.46
23	f	103	LHG	O8-C23-C24	2.77	120.27	111.83
22	f	101	CDL	OA8-CA7-C31	2.70	120.08	111.83
23	f	102	LHG	O8-C23-C24	2.69	120.05	111.83
21	E	600	ADP	C5-N7-C8	2.69	107.68	103.45
21	F	600	ADP	C4-N9-C8	2.68	108.55	105.74
21	F	600	ADP	C5-N7-C8	2.68	107.66	103.45
21	F	600	ADP	C3'-C2'-C1'	2.67	106.52	101.46
22	b	301	CDL	OA8-CA7-C31	2.66	119.96	111.83
21	E	600	ADP	C3'-C2'-C1'	2.56	106.31	101.46
19	C	600	ATP	C5-N7-C8	2.54	107.44	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	f	101	CDL	OB8-CB7-C71	2.53	119.56	111.83
21	D	600	ADP	C4-N9-C8	2.53	108.40	105.74
19	B	600	ATP	C5-N7-C8	2.53	107.43	103.45
21	D	600	ADP	C5-N7-C8	2.51	107.40	103.45
23	f	102	LHG	C11-C10-C9	-2.51	101.67	114.37
22	b	301	CDL	OB8-CB7-C71	2.50	119.44	111.83
19	A	600	ATP	C5-N7-C8	2.41	107.24	103.45
19	B	600	ATP	N9-C8-N7	-2.35	110.61	113.94
19	A	600	ATP	C3'-C2'-C1'	2.31	105.84	101.46
23	f	103	LHG	C11-C10-C9	-2.31	102.71	114.37
21	E	600	ADP	N9-C8-N7	-2.27	110.72	113.94
22	b	302	CDL	CA4-OA6-CA5	-2.26	112.40	117.80
19	C	600	ATP	N9-C8-N7	-2.25	110.74	113.94
19	C	600	ATP	C2'-C1'-N9	-2.23	107.77	113.30
21	F	600	ADP	N9-C8-N7	-2.23	110.78	113.94
19	C	600	ATP	O4'-C1'-N9	2.17	112.25	108.09
21	E	600	ADP	C6-C5-N7	2.16	136.26	132.09
23	f	102	LHG	C27-C26-C25	-2.16	103.46	114.37
19	C	600	ATP	C3'-C2'-C1'	2.15	105.53	101.46
21	F	600	ADP	C6-C5-N7	2.15	136.23	132.09
19	A	600	ATP	N9-C8-N7	-2.11	110.94	113.94
23	f	102	LHG	C18-C17-C16	-2.09	103.82	114.37
21	D	600	ADP	C2-N1-C6	2.08	122.15	118.73
19	A	600	ATP	C2-N1-C6	2.08	122.14	118.73
21	D	600	ADP	N9-C8-N7	-2.07	111.00	113.94
21	E	600	ADP	C2-N1-C6	2.04	122.08	118.73
21	D	600	ADP	C6-C5-N7	2.04	136.01	132.09
23	f	103	LHG	C20-C19-C18	-2.03	104.10	114.37
19	B	600	ATP	C2-N1-C6	2.03	122.06	118.73

There are no chirality outliers.

All (159) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	C	600	ATP	C5'-O5'-PA-O1A
21	D	600	ADP	C5'-O5'-PA-O3A
21	E	600	ADP	PB-O3A-PA-O5'
21	E	600	ADP	C5'-O5'-PA-O1A
21	F	600	ADP	C5'-O5'-PA-O1A
21	F	600	ADP	C5'-O5'-PA-O2A
21	F	600	ADP	C5'-O5'-PA-O3A
22	f	101	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
22	b	301	CDL	C11-CA5-OA6-CA4
22	b	301	CDL	CB2-OB2-PB2-OB3
22	b	301	CDL	CB2-OB2-PB2-OB4
22	b	301	CDL	CB2-OB2-PB2-OB5
22	b	301	CDL	CB3-OB5-PB2-OB2
22	b	301	CDL	CB3-OB5-PB2-OB3
22	b	301	CDL	OB5-CB3-CB4-OB6
22	b	301	CDL	C51-CB5-OB6-CB4
22	b	302	CDL	C1-CA2-OA2-PA1
22	b	302	CDL	CA2-OA2-PA1-OA3
22	b	302	CDL	CA2-OA2-PA1-OA4
22	b	302	CDL	CA2-OA2-PA1-OA5
22	b	302	CDL	CB2-OB2-PB2-OB3
22	b	302	CDL	CB2-OB2-PB2-OB4
22	b	302	CDL	CB2-OB2-PB2-OB5
22	b	302	CDL	CB3-OB5-PB2-OB2
22	b	302	CDL	CB3-OB5-PB2-OB3
22	b	302	CDL	CB3-OB5-PB2-OB4
23	f	102	LHG	C3-O3-P-O4
23	f	102	LHG	C3-O3-P-O6
23	f	103	LHG	C1-C2-C3-O3
22	b	301	CDL	OA7-CA5-OA6-CA4
22	b	301	CDL	OB7-CB5-OB6-CB4
22	f	101	CDL	C31-CA7-OA8-CA6
22	b	301	CDL	O1-C1-CA2-OA2
23	f	103	LHG	O2-C2-C3-O3
22	f	101	CDL	OA9-CA7-OA8-CA6
22	f	101	CDL	C1-CB2-OB2-PB2
22	b	301	CDL	C1-CA2-OA2-PA1
22	b	301	CDL	CB5-C51-C52-C53
22	b	302	CDL	CA5-C11-C12-C13
23	f	103	LHG	C7-C8-C9-C10
22	f	101	CDL	CB5-C51-C52-C53
22	f	101	CDL	CA5-C11-C12-C13
22	b	301	CDL	CB2-C1-CA2-OA2
21	F	600	ADP	O4'-C4'-C5'-O5'
22	b	302	CDL	CB4-CB3-OB5-PB2
23	f	102	LHG	O1-C1-C2-C3
23	f	103	LHG	O1-C1-C2-C3
22	b	302	CDL	C11-CA5-OA6-CA4
22	b	301	CDL	C19-C20-C21-C22
22	b	301	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	f	103	LHG	C28-C29-C30-C31
22	f	101	CDL	C75-C76-C77-C78
21	F	600	ADP	C3'-C4'-C5'-O5'
23	f	102	LHG	C7-C8-C9-C10
22	f	101	CDL	C73-C74-C75-C76
22	b	301	CDL	C40-C41-C42-C43
22	b	302	CDL	OA7-CA5-OA6-CA4
22	b	302	CDL	C73-C74-C75-C76
22	f	101	CDL	C71-C72-C73-C74
22	b	302	CDL	C60-C61-C62-C63
22	b	301	CDL	C37-C38-C39-C40
22	b	302	CDL	C13-C14-C15-C16
22	b	302	CDL	C54-C55-C56-C57
23	f	103	LHG	C5-C4-O6-P
22	f	101	CDL	OB5-CB3-CB4-CB6
22	f	101	CDL	C54-C55-C56-C57
22	b	302	CDL	C71-C72-C73-C74
22	f	101	CDL	C12-C13-C14-C15
23	f	102	LHG	C13-C14-C15-C16
23	f	103	LHG	C31-C32-C33-C34
22	f	101	CDL	CA7-C31-C32-C33
22	f	101	CDL	C71-CB7-OB8-CB6
22	b	301	CDL	C71-C72-C73-C74
22	b	302	CDL	OB6-CB4-CB6-OB8
23	f	102	LHG	C27-C28-C29-C30
22	b	301	CDL	C17-C18-C19-C20
22	b	301	CDL	OB5-CB3-CB4-CB6
23	f	102	LHG	C4-C5-C6-O8
23	f	103	LHG	C14-C15-C16-C17
22	b	302	CDL	C11-C12-C13-C14
22	f	101	CDL	C13-C14-C15-C16
22	f	101	CDL	OB9-CB7-OB8-CB6
22	b	302	CDL	C16-C17-C18-C19
22	f	101	CDL	C74-C75-C76-C77
23	f	103	LHG	O6-C4-C5-C6
22	b	302	CDL	C53-C54-C55-C56
23	f	103	LHG	O6-C4-C5-O7
23	f	103	LHG	C15-C16-C17-C18
23	f	103	LHG	C13-C14-C15-C16
22	f	101	CDL	C52-C53-C54-C55
23	f	102	LHG	O1-C1-C2-O2
22	f	101	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
22	b	302	CDL	C51-C52-C53-C54
22	f	101	CDL	OB5-CB3-CB4-OB6
22	b	302	CDL	OB5-CB3-CB4-OB6
22	f	101	CDL	C51-CB5-OB6-CB4
22	f	101	CDL	C56-C57-C58-C59
23	f	102	LHG	O7-C5-C6-O8
22	f	101	CDL	C77-C78-C79-C80
19	C	600	ATP	C5'-O5'-PA-O2A
19	C	600	ATP	C5'-O5'-PA-O3A
21	D	600	ADP	C5'-O5'-PA-O1A
21	E	600	ADP	C5'-O5'-PA-O3A
22	f	101	CDL	CA3-OA5-PA1-OA3
22	b	301	CDL	CA2-OA2-PA1-OA3
22	b	301	CDL	CA2-OA2-PA1-OA4
22	b	301	CDL	CA2-OA2-PA1-OA5
22	b	301	CDL	CA3-OA5-PA1-OA4
23	f	102	LHG	C2-C3-O3-P
22	b	301	CDL	C73-C74-C75-C76
23	f	103	LHG	O10-C23-O8-C6
22	b	302	CDL	CB3-CB4-CB6-OB8
23	f	103	LHG	C32-C33-C34-C35
23	f	103	LHG	C11-C12-C13-C14
22	b	301	CDL	C13-C14-C15-C16
22	b	301	CDL	C72-C73-C74-C75
22	b	301	CDL	C52-C53-C54-C55
19	C	600	ATP	PB-O3B-PG-O1G
22	b	301	CDL	CA3-CA4-CA6-OA8
22	f	101	CDL	CA4-CA6-OA8-CA7
22	f	101	CDL	C1-CA2-OA2-PA1
22	f	101	CDL	CA4-CA3-OA5-PA1
22	b	301	CDL	C1-CB2-OB2-PB2
22	f	101	CDL	C39-C40-C41-C42
22	b	302	CDL	OB5-CB3-CB4-CB6
23	f	103	LHG	C34-C35-C36-C37
22	f	101	CDL	C14-C15-C16-C17
22	b	301	CDL	C31-CA7-OA8-CA6
22	b	301	CDL	CA5-C11-C12-C13
22	f	101	CDL	C53-C54-C55-C56
22	b	301	CDL	OA9-CA7-OA8-CA6
22	b	302	CDL	C12-C11-CA5-OA6
22	f	101	CDL	C60-C61-C62-C63
23	f	102	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	f	101	CDL	C31-C32-C33-C34
22	f	101	CDL	C76-C77-C78-C79
22	b	302	CDL	C59-C60-C61-C62
22	b	301	CDL	CB3-CB4-CB6-OB8
22	b	301	CDL	C31-C32-C33-C34
22	f	101	CDL	C16-C17-C18-C19
23	f	102	LHG	C10-C11-C12-C13
22	f	101	CDL	OA7-CA5-OA6-CA4
22	b	302	CDL	C33-C34-C35-C36
22	f	101	CDL	C11-C12-C13-C14
22	b	301	CDL	C53-C54-C55-C56
23	f	102	LHG	C24-C25-C26-C27
22	b	302	CDL	CB6-CB4-OB6-CB5
22	b	301	CDL	CB4-CB6-OB8-CB7
22	b	301	CDL	CA4-CA3-OA5-PA1
23	f	103	LHG	C29-C30-C31-C32
23	f	103	LHG	O1-C1-C2-O2
22	b	301	CDL	OA6-CA4-CA6-OA8
22	f	101	CDL	C12-C11-CA5-OA6
22	f	101	CDL	C11-CA5-OA6-CA4
19	B	600	ATP	PB-O3A-PA-O2A
21	E	600	ADP	O4'-C4'-C5'-O5'
22	b	301	CDL	C32-C31-CA7-OA8
23	f	102	LHG	O9-C7-C8-C9
22	b	301	CDL	C35-C36-C37-C38

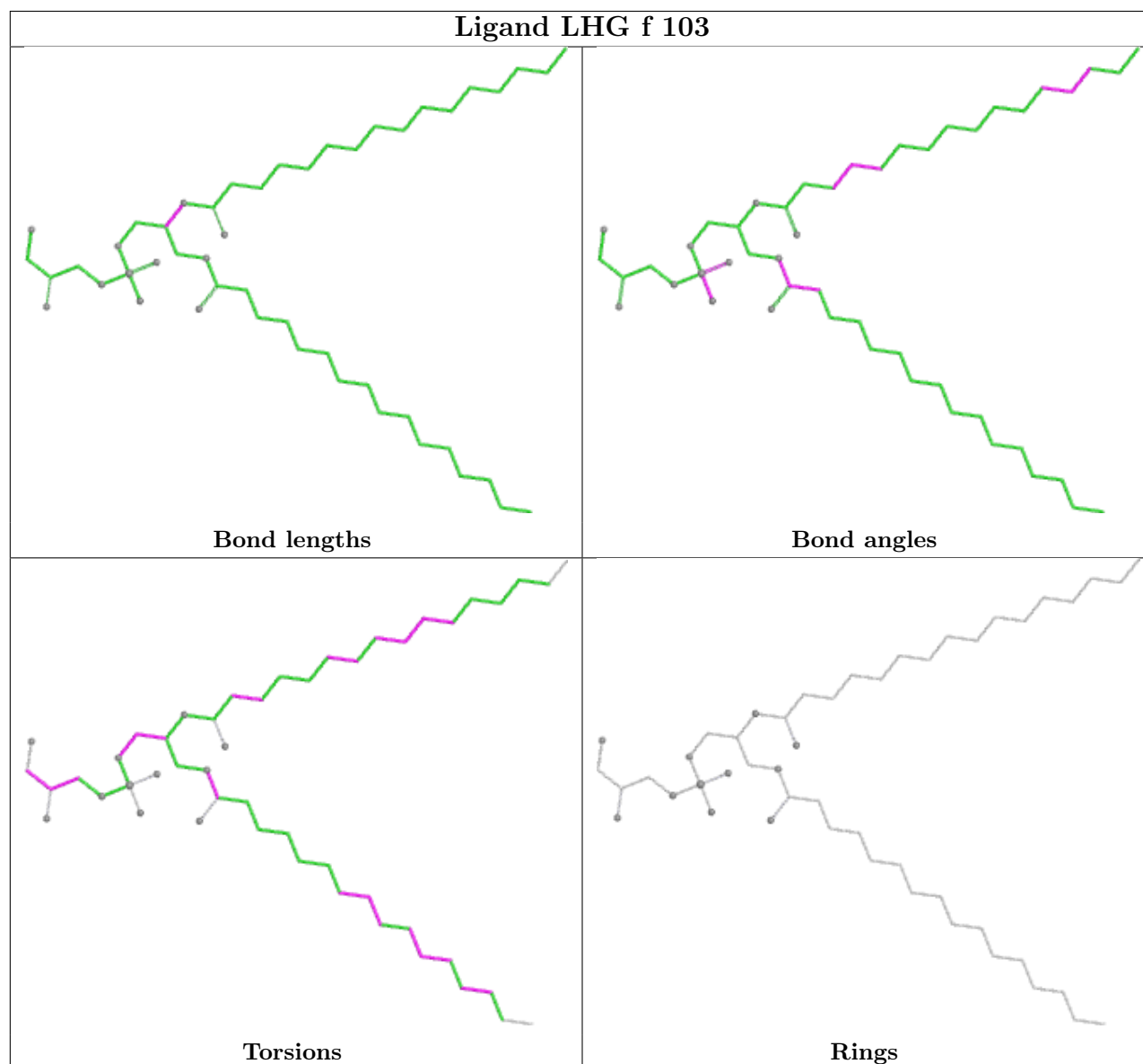
There are no ring outliers.

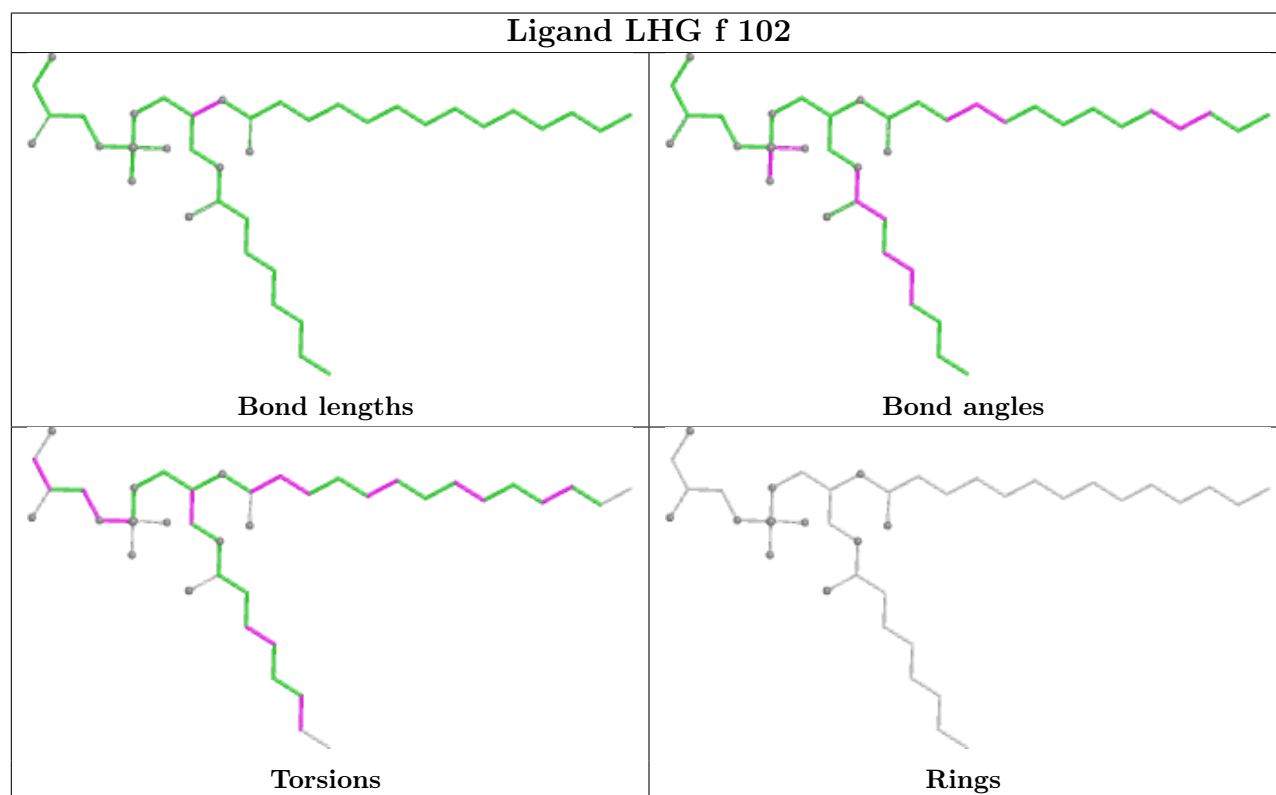
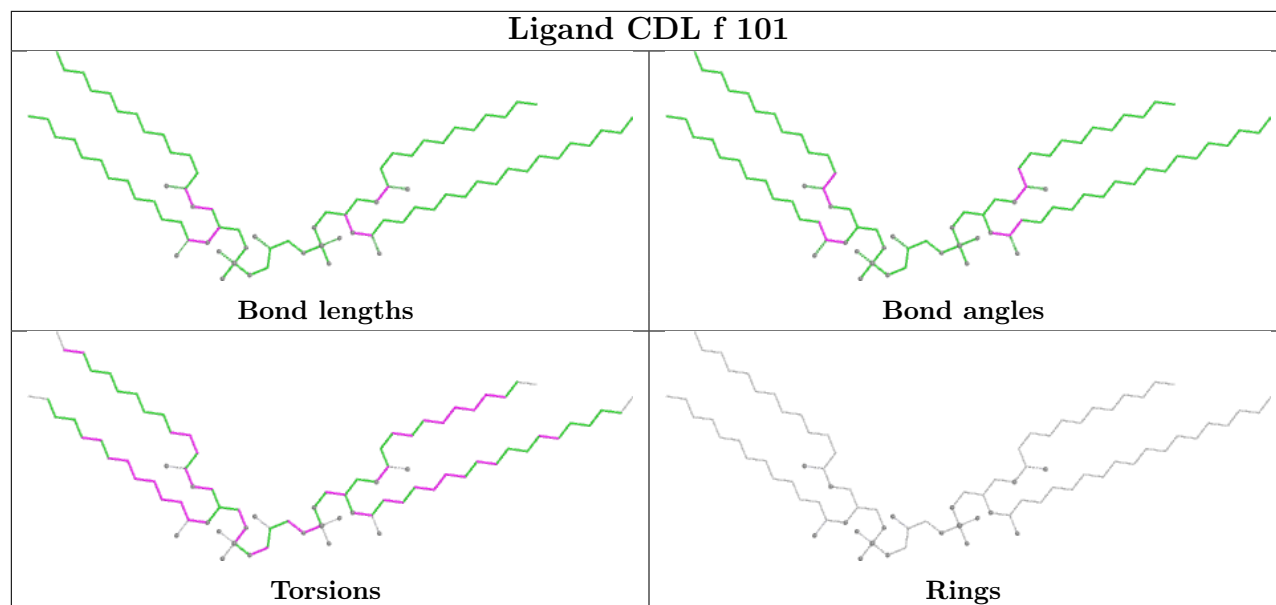
8 monomers are involved in 18 short contacts:

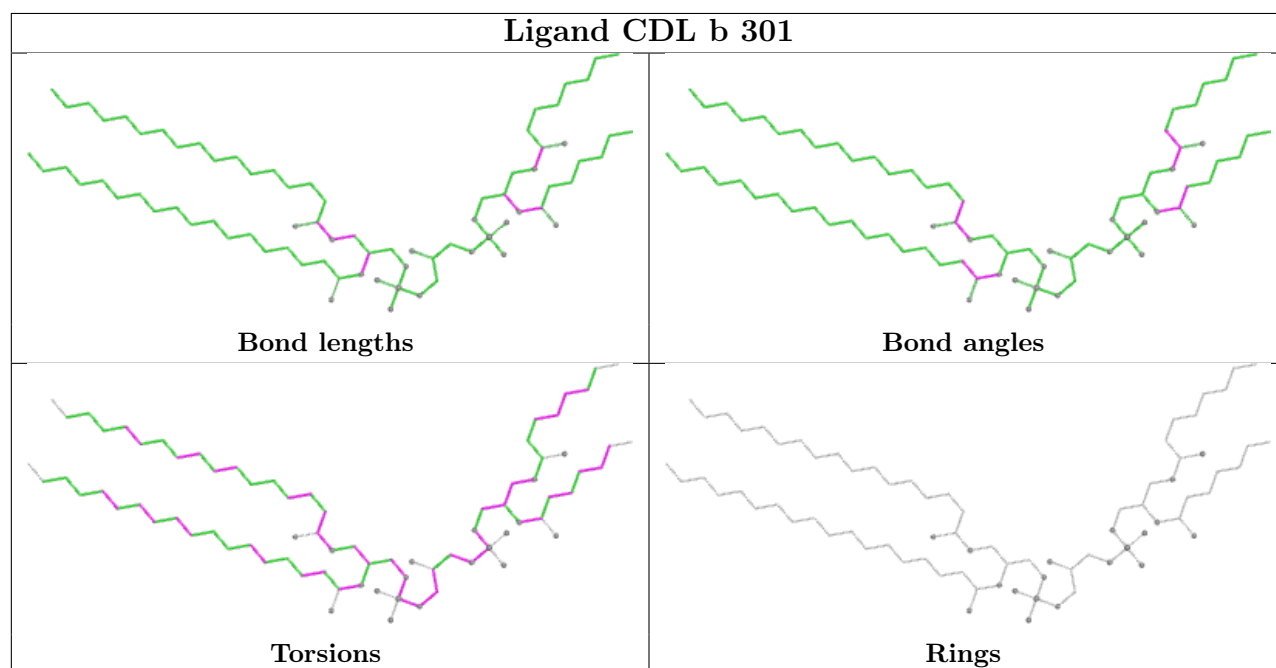
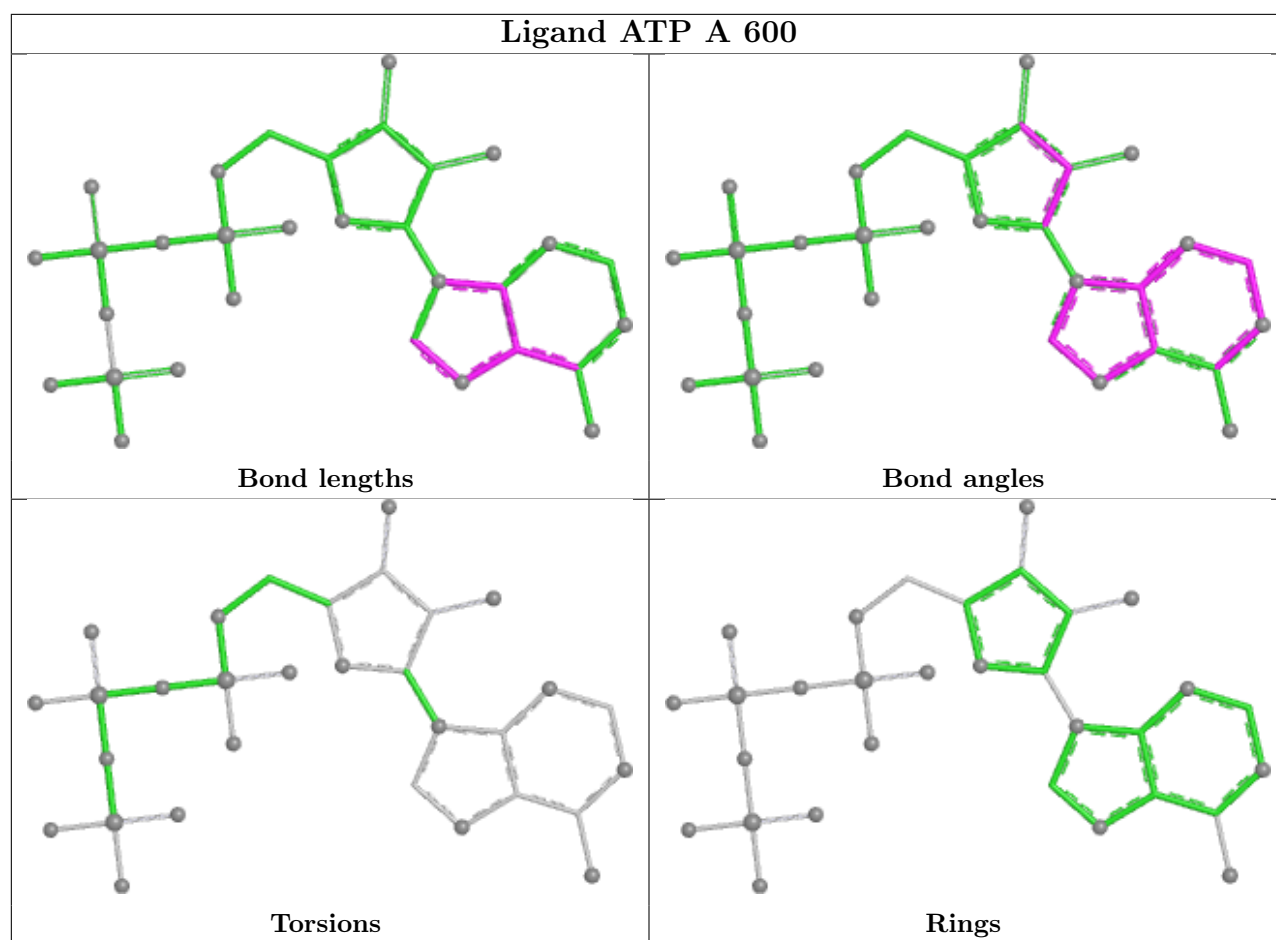
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	f	101	CDL	4	0
23	f	102	LHG	2	0
22	b	301	CDL	4	0
22	b	302	CDL	2	0
21	E	600	ADP	2	0
21	D	600	ADP	1	0
19	C	600	ATP	1	0
19	B	600	ATP	2	0

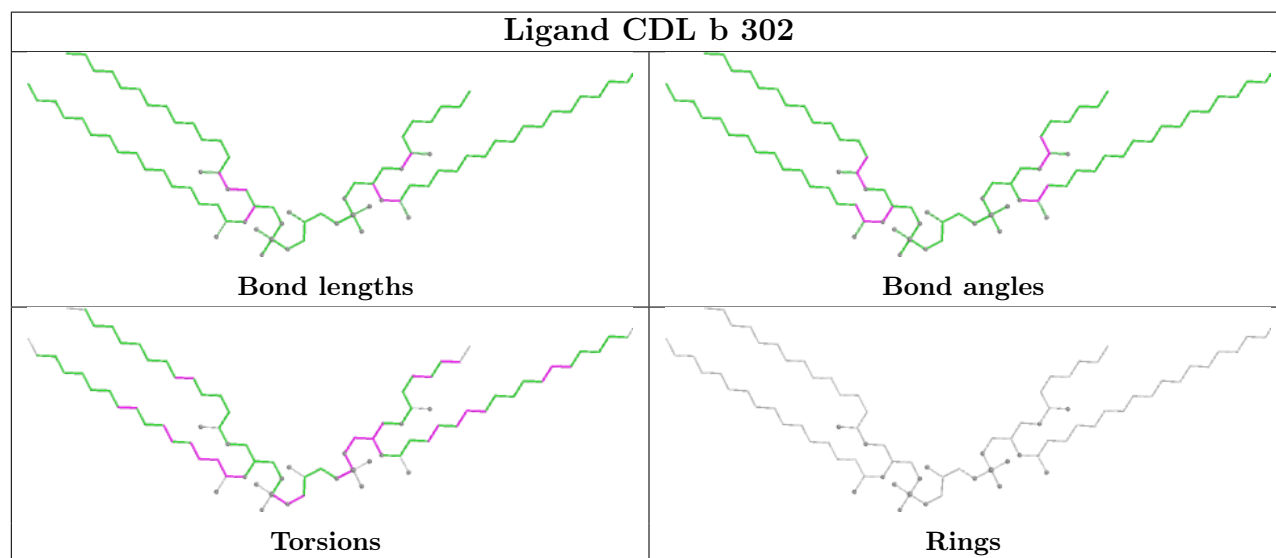
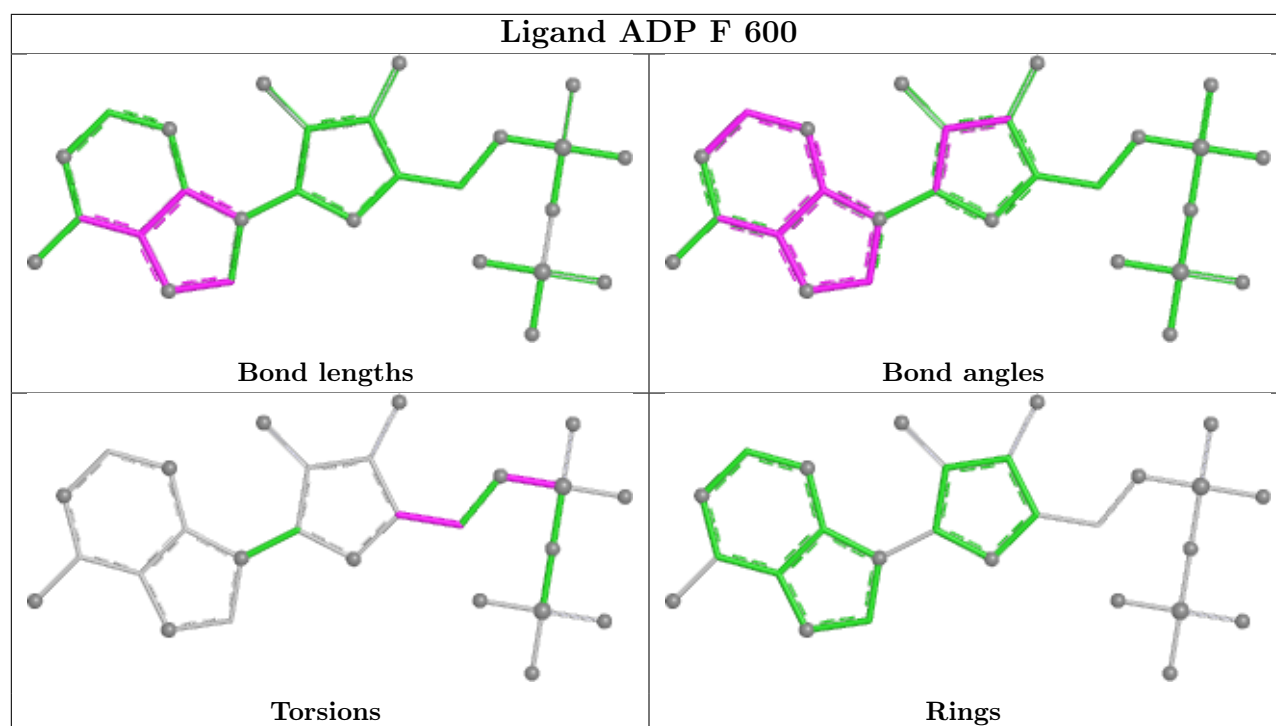
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

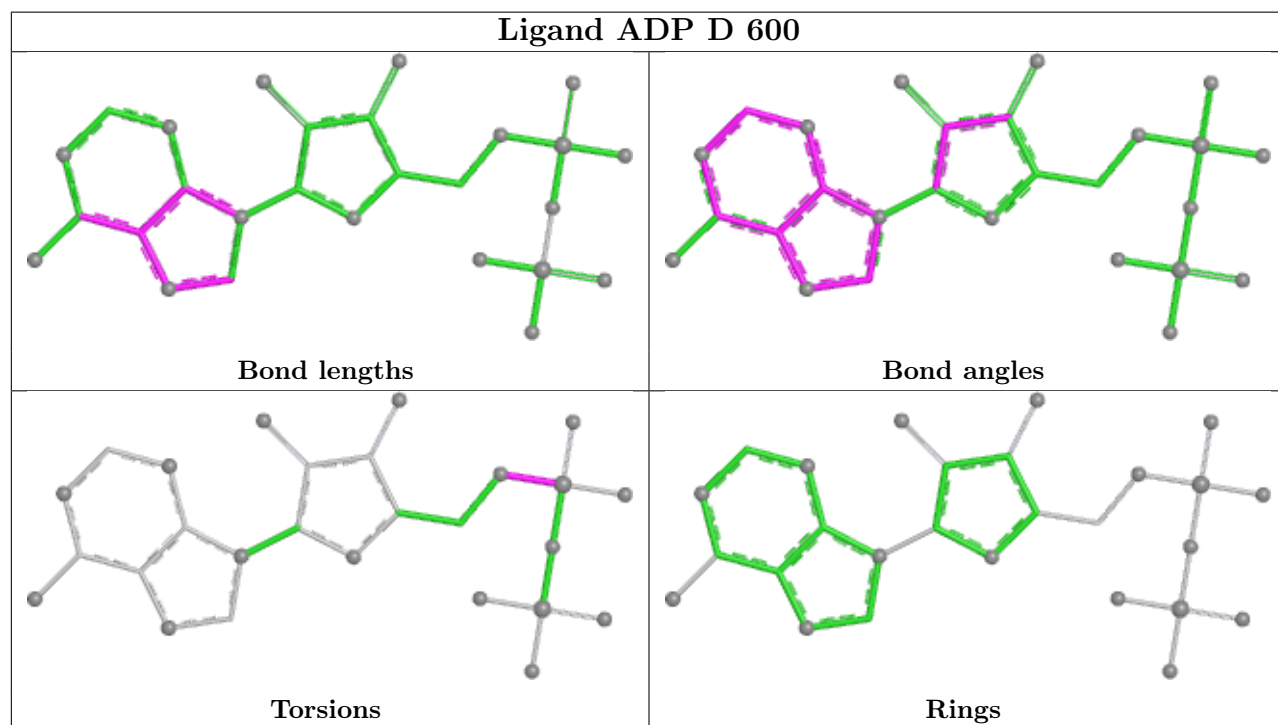
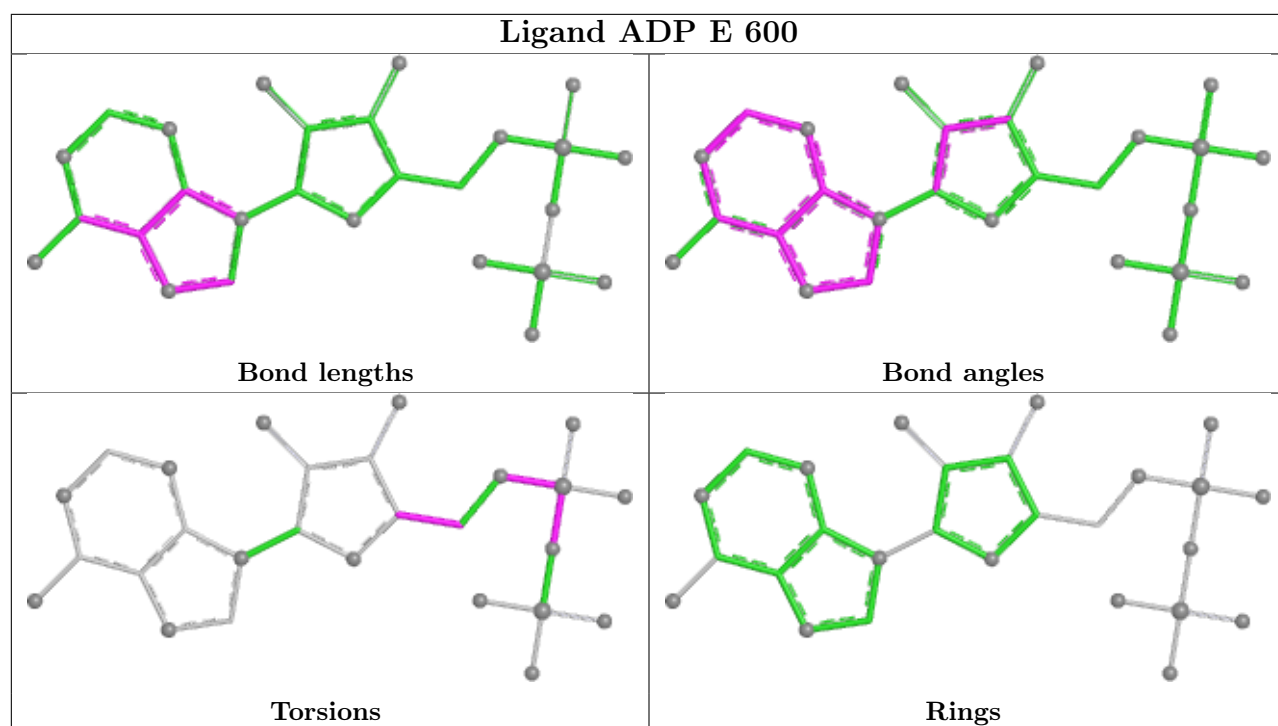
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

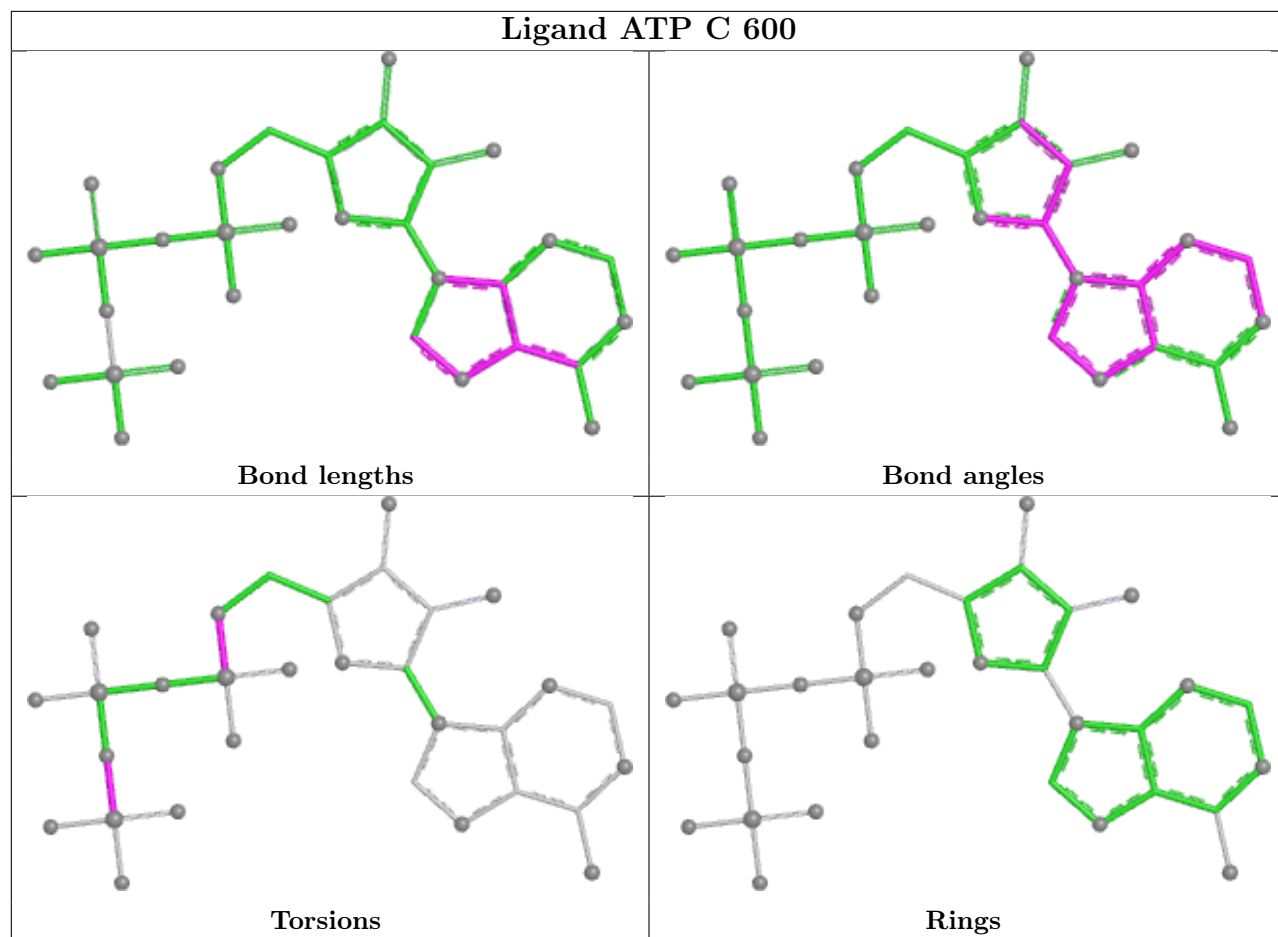


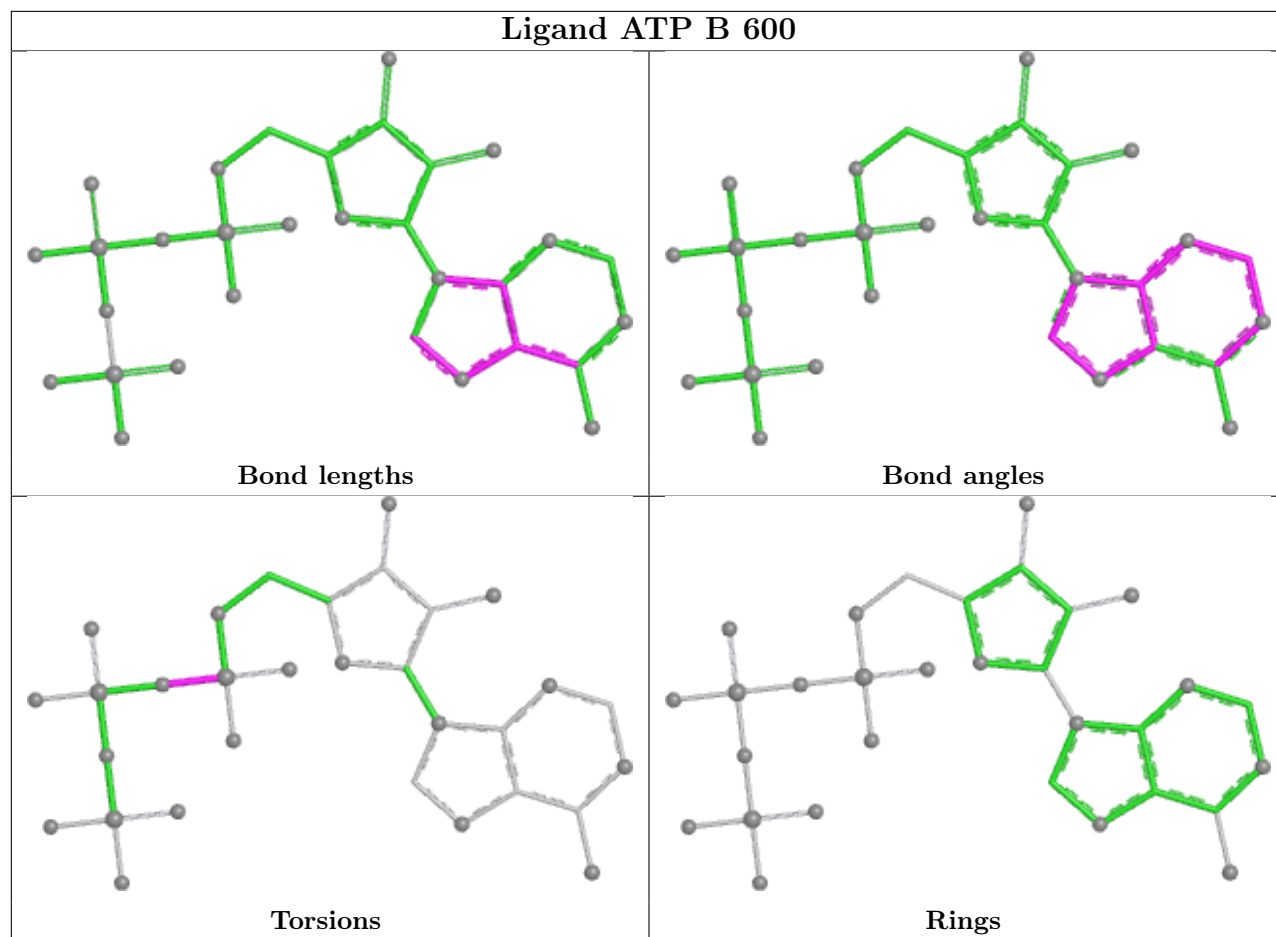












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

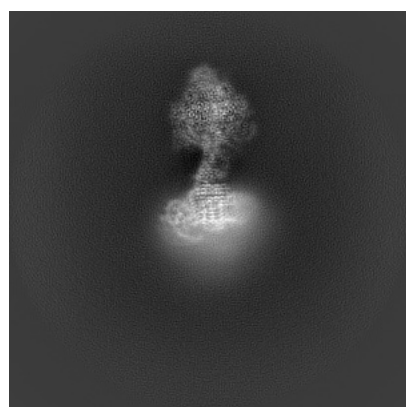
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11369. These allow visual inspection of the internal detail of the map and identification of artifacts.

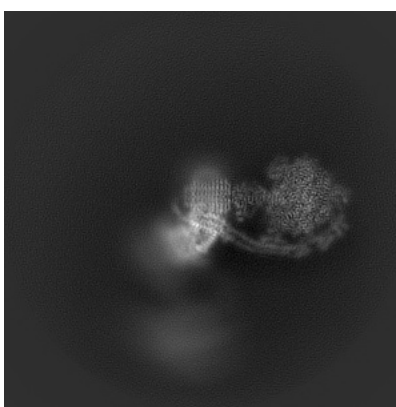
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

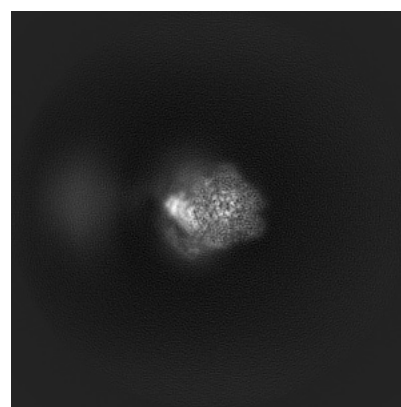
6.1.1 Primary map



X



Y

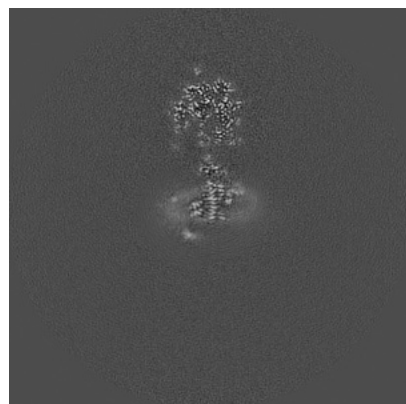


Z

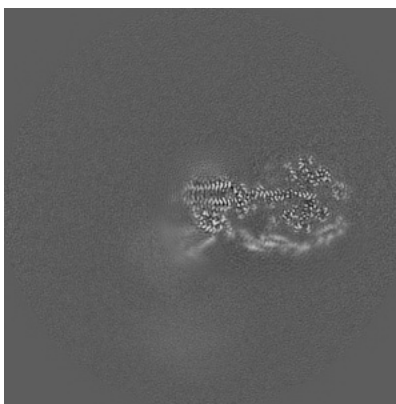
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

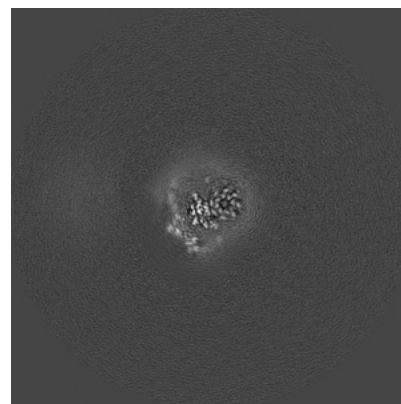
6.2.1 Primary map



X Index: 250



Y Index: 250

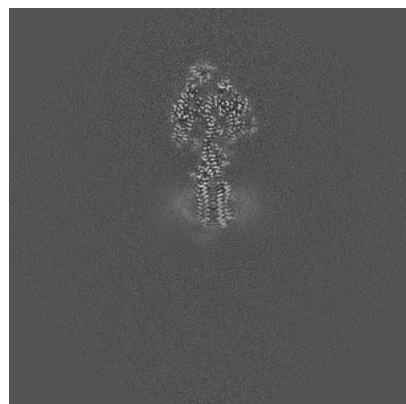


Z Index: 250

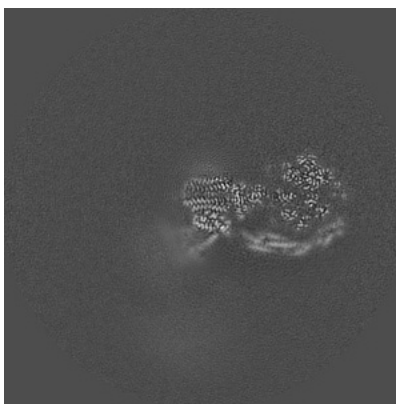
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

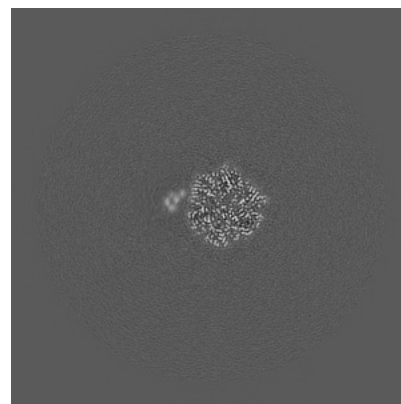
6.3.1 Primary map



X Index: 264



Y Index: 253

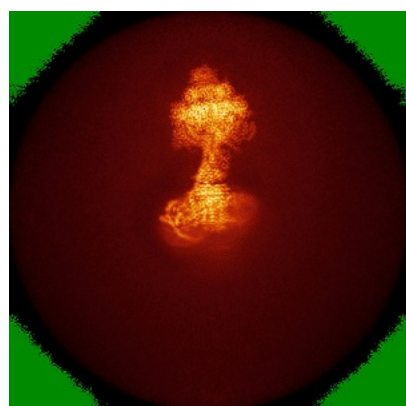


Z Index: 375

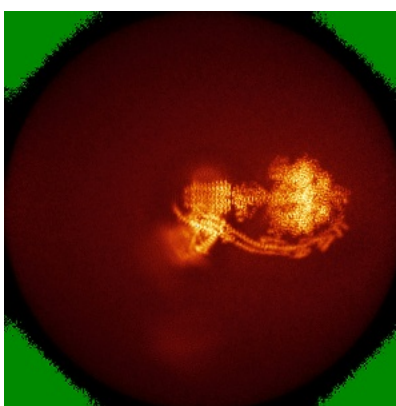
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

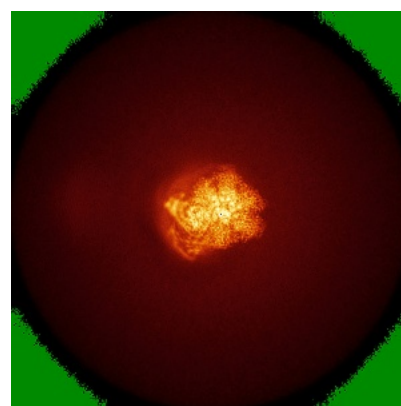
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

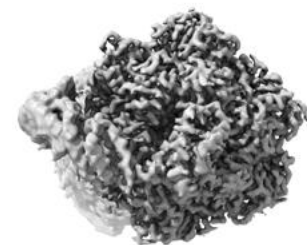
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.92. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

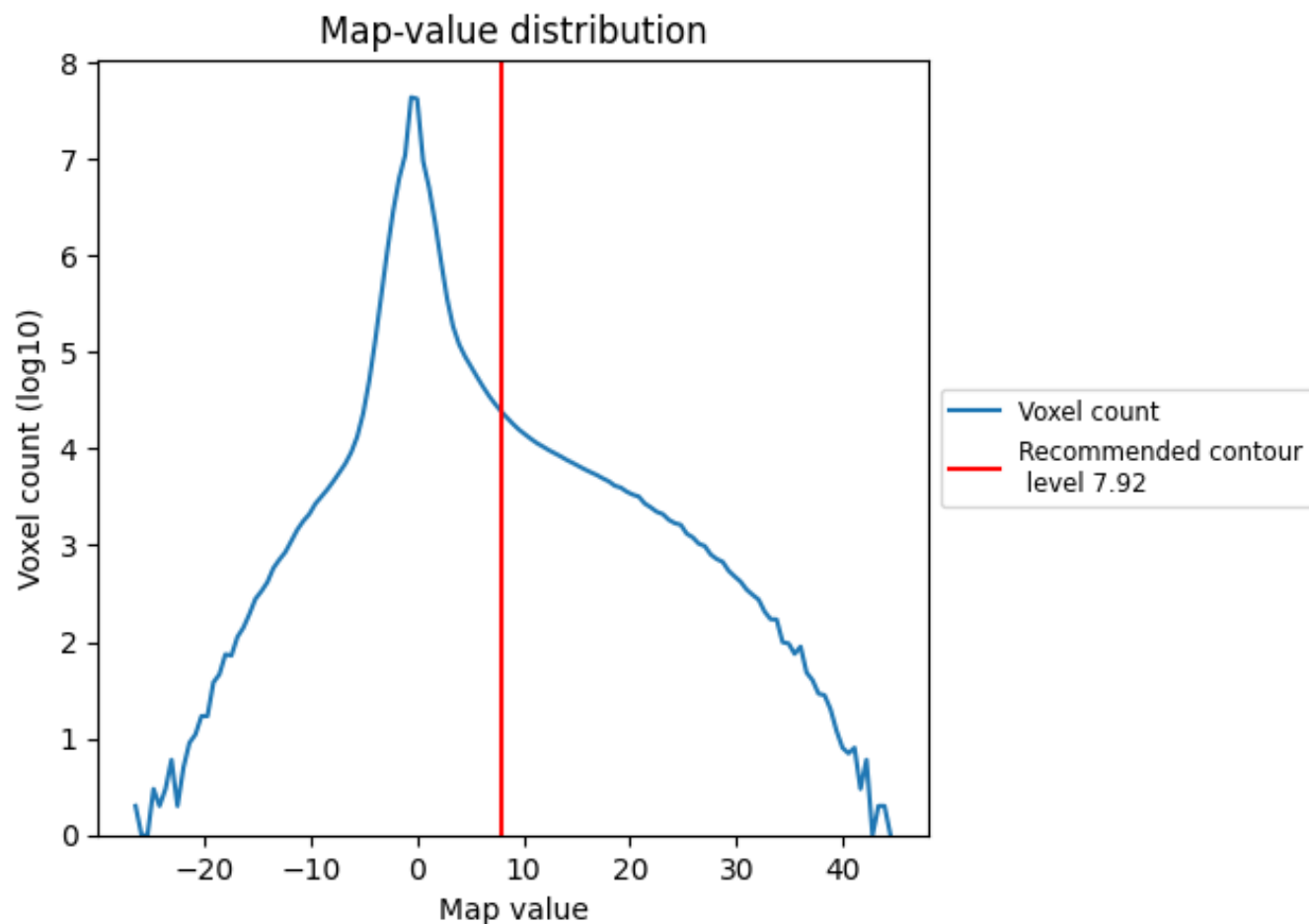
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

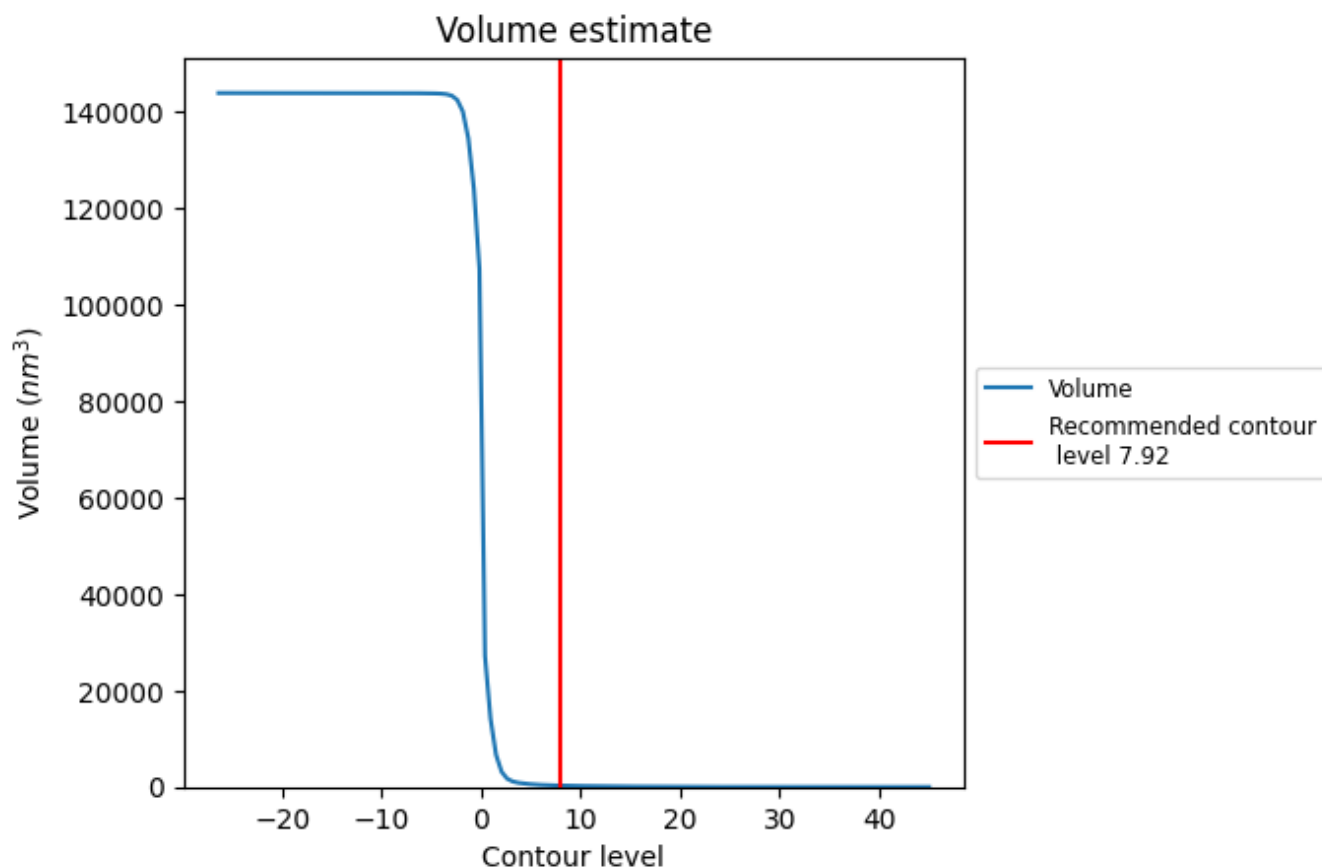
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

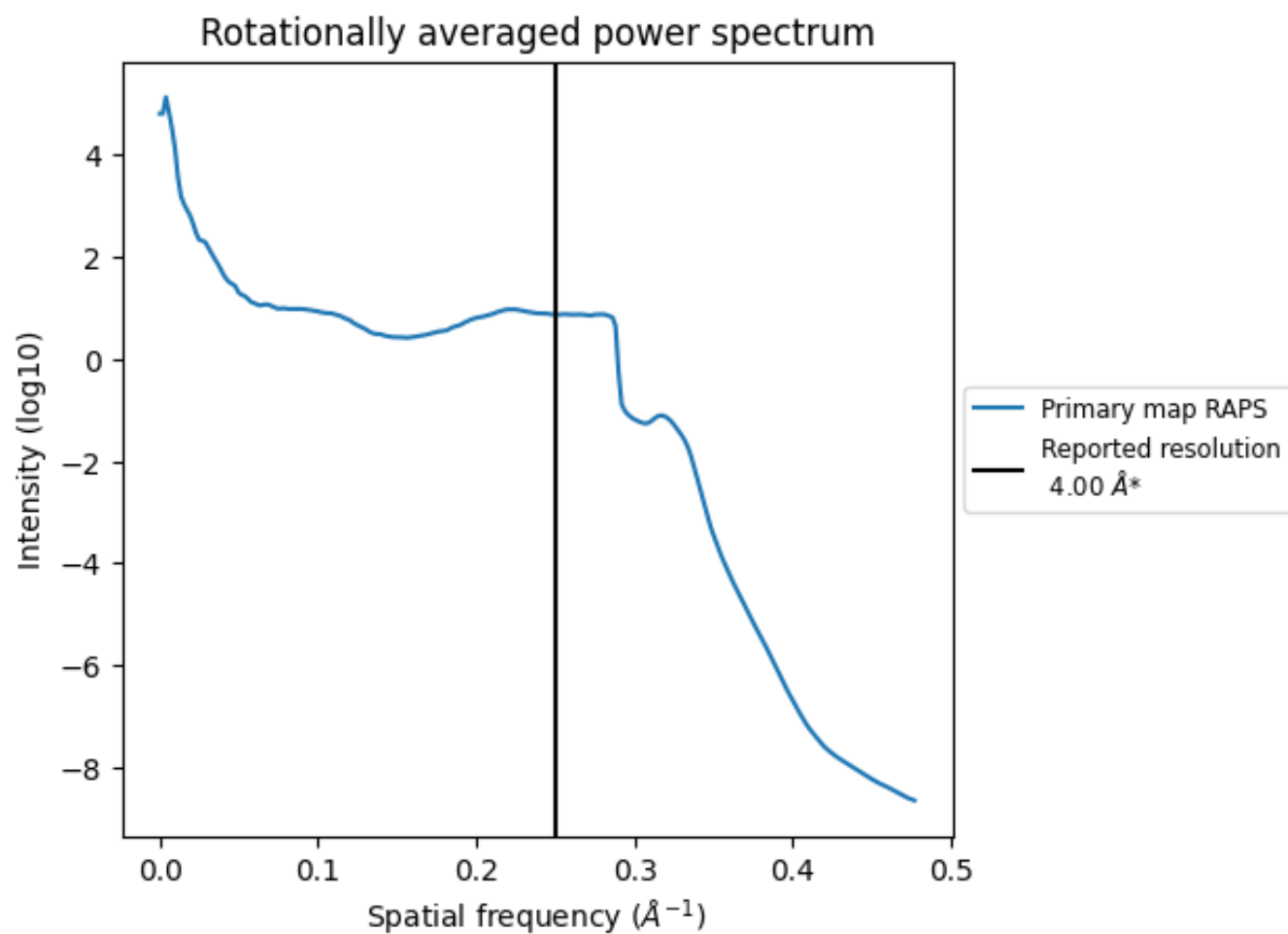
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 281 nm³; this corresponds to an approximate mass of 254 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

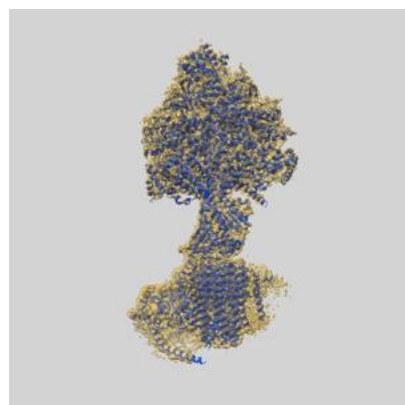
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

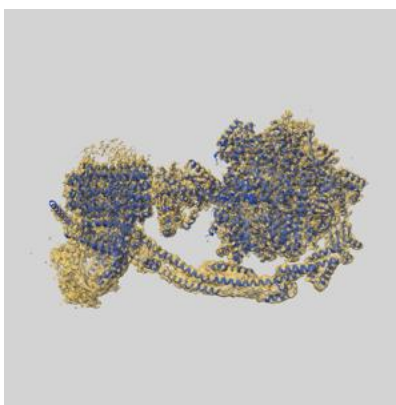
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11369 and PDB model 6ZQN. Per-residue inclusion information can be found in section 3 on page 11.

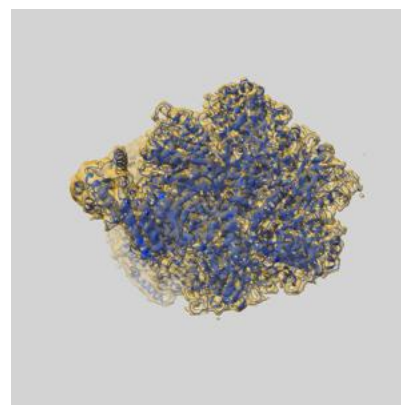
9.1 Map-model overlay [i](#)



X



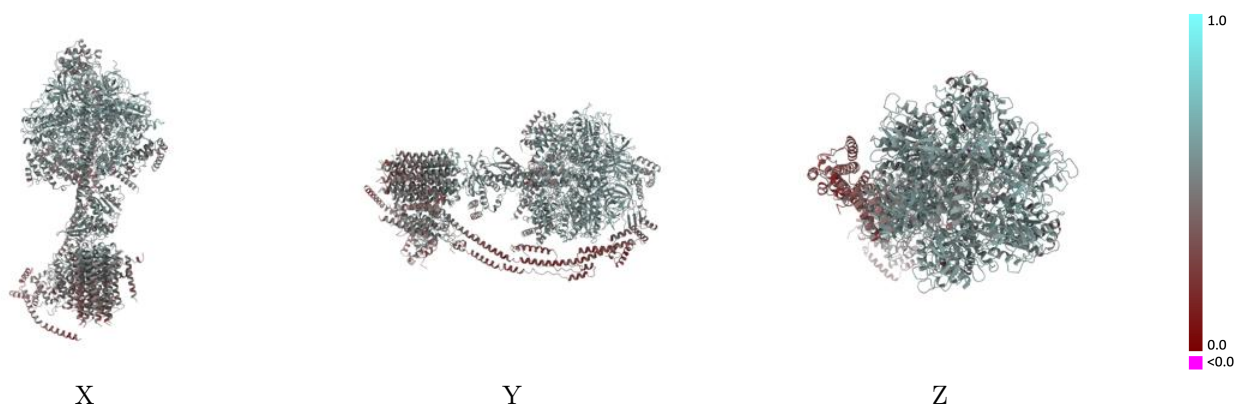
Y



Z

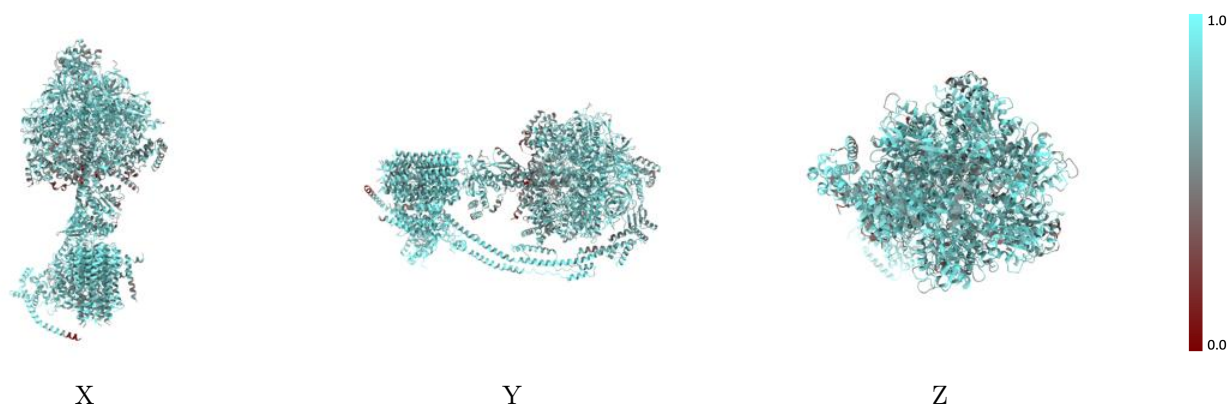
The images above show the 3D surface view of the map at the recommended contour level 7.92 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



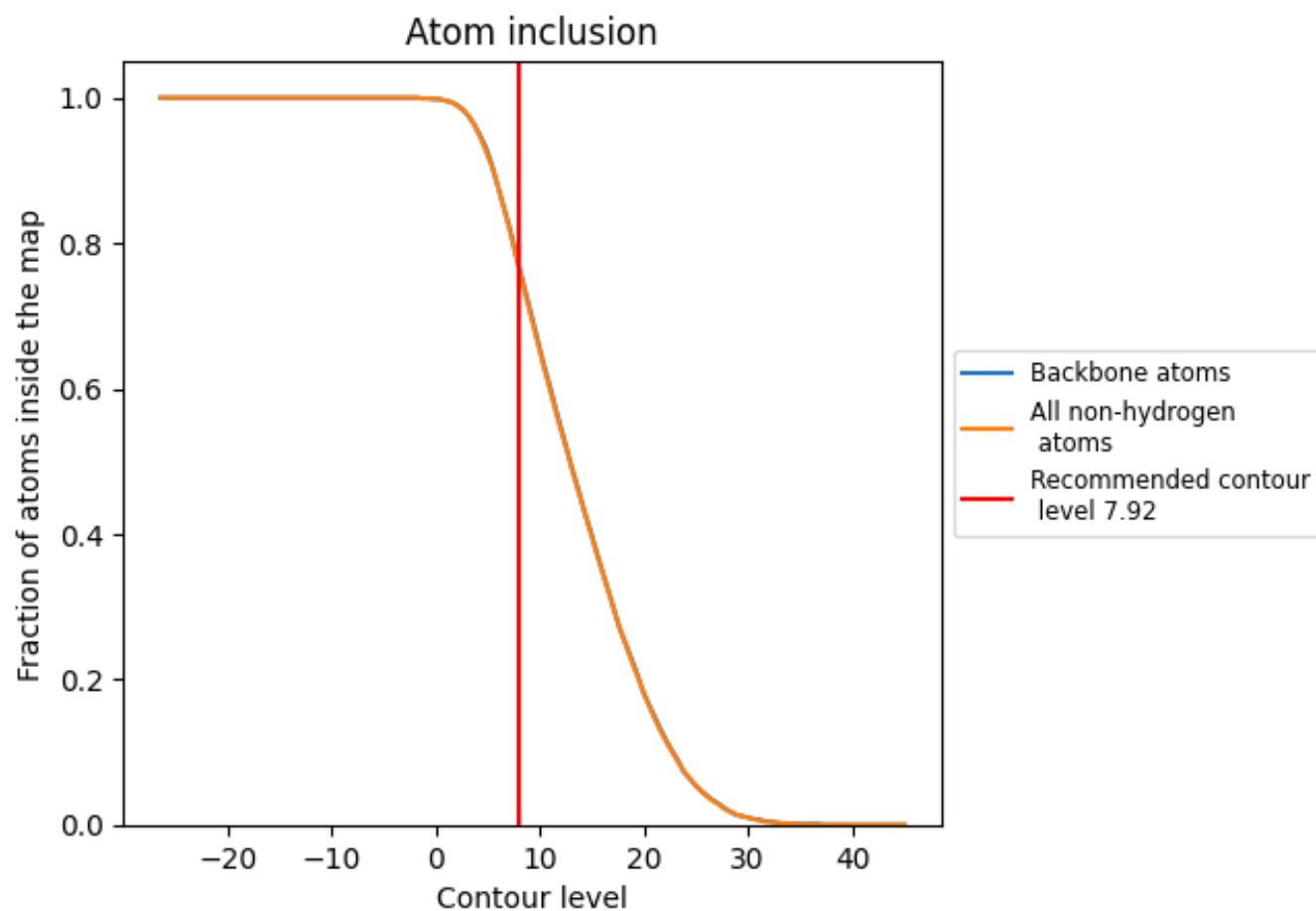
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7.92).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (7.92) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7690	 0.5020
8	 0.8860	 0.4780
A	 0.7730	 0.5470
B	 0.7510	 0.5480
C	 0.7510	 0.5460
D	 0.7740	 0.5570
E	 0.7410	 0.5470
F	 0.7730	 0.5560
G	 0.7190	 0.5290
H	 0.7940	 0.5060
I	 0.7240	 0.5290
J	 0.5830	 0.4990
K	 0.7850	 0.4510
L	 0.8090	 0.4640
M	 0.8090	 0.4660
N	 0.8160	 0.4710
O	 0.7900	 0.4680
P	 0.8110	 0.4750
Q	 0.7360	 0.4010
R	 0.7820	 0.4600
S	 0.6810	 0.4950
a	 0.8680	 0.4630
b	 0.8390	 0.3740
d	 0.8630	 0.3290
e	 0.7730	 0.3650
f	 0.8730	 0.4560
g	 0.9030	 0.3370
h	 0.7020	 0.2740
j	 0.8360	 0.3930
k	 0.7080	 0.3970

